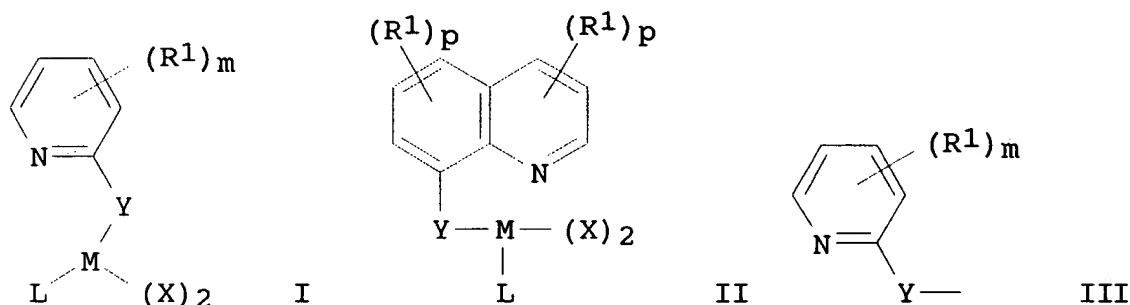


L30 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 1998 ACS  
 AN 1996:758983 HCAPLUS  
 DN 126:31794  
 TI Transition metal catalysts based on bidentate ligands containing  
 pyridine or quinoline moiety  
 IN **Nagy, Sandor; Krishnamurti, Ramesh; Tyrell,  
 John A.; Cribbs, Leonard V.; Cocoman, Mary**  
 PA Occidental Chemical Corporation, USA  
 SO PCT Int. Appl., 24 pp.  
 CODEN: PIXXD2  
 PI WO 9633202 A2 961024  
 DS W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP,  
 KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NZ, PL, RO,  
 RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN  
 RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,  
 GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG  
 AI WO 96-US3656 960318  
 PRAI US 95-423232 950417  
 DT Patent  
 LA English  
 IC ICM C07F017-00  
 ICS B01J031-122; C08F010-00  
 CC 35-3 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 29  
 OS MARPAT 126:31794  
 GI



AB Transition metal catalysts for  $\alpha$ -olefin polymn. are characterized by having bidentate ligands contg. pyridine or quinoline moiety and have general structure I and II [Y = O, S, NR, (CR<sub>2</sub>)<sub>n</sub>NR, (CR<sub>2</sub>)<sub>n</sub>O; R = H, C1-6 alkyl; R' = R, C1-6 alkoxy, C6-16 aryl, halogen, CF<sub>3</sub>; M = Ti, Zr, Hf; X = halogen, C1-6 alkyl, C1-6 alkoxy, NR<sub>2</sub>; L = X, cyclopentadienyl, C1-6 alkyl-substituted cyclopentadienyl, indenyl, fluorenyl, III; m = 0-4; n = 1-4, p = 0-3]. Thus polyethylene with Mw/Mn 3.67 and melt flow rate 10.2 was produced by using a catalyst system including 8-quinolinoxytitanium trichloride, which was prepd. from 8-hydroxyquinoline and TiCl<sub>4</sub>, and

Me aluminoxanes in a molar ratio of Al/Ti = 1074; the catalyst productivity was 167.9 kg/g Ti/h.

ST polymn catalyst olefin alpha; pyridine quinoline ligand transition metal catalyst

IT Coordination polymerization catalysts  
 (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT Methyl aluminoxanes  
 (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT Linear low-density polyethylenes  
 (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT 72-80-0 142-08-5, 2-Pyridinone 148-24-3, 8-Hydroxyquinoline, reactions 1270-98-0, Cyclopentadienyltitanium trichloride 7550-45-0, Titanium tetrachloride, reactions 34767-44-7, Cyclopentadienylzirconium trichloride  
 (prepn. of transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety)

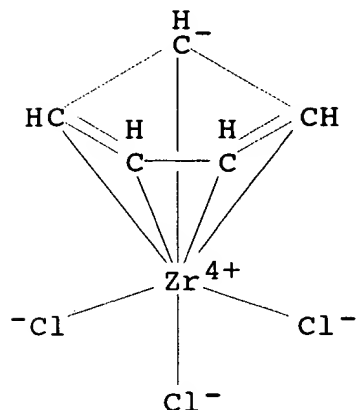
IT 15614-57-0P 184534-40-5P 184534-41-6P 184534-42-7P  
 184534-43-8P 184534-44-9P  
 (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT 9002-88-4P, Polyethylene 25087-34-7P  
 (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

=&gt; d 131 scan

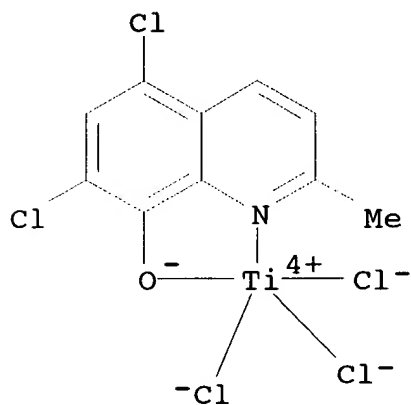
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN Zirconium, trichloro(.eta.5-2,4-cyclopentadien-1-yl)- (9CI)  
 MF C5 H5 Cl3 Zr  
 CI CCS, COM

← (Compounds cited  
 in the above  
 abstracts)

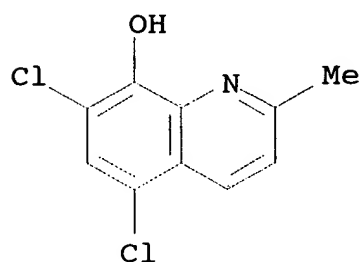


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

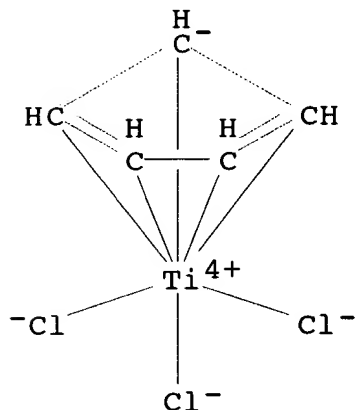
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN Titanium, trichloro(5,7-dichloro-2-methyl-8-quinolinolato-  
 .kappa.N1,.kappa.O8)- (9CI)  
 MF C10 H6 Cl5 N O Ti  
 CI CCS



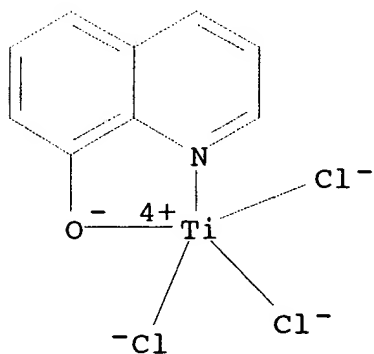
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN 8-Quinolinol, 5,7-dichloro-2-methyl- (6CI, 7CI, 8CI, 9CI)  
 MF C10 H7 Cl2 N O  
 CI COM



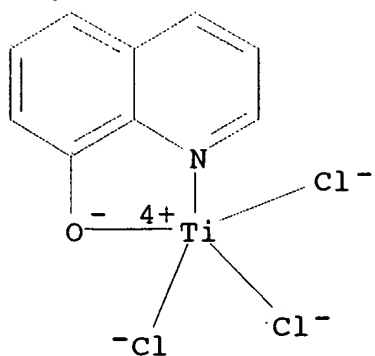
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
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 MF C5 H5 Cl3 Ti  
 CI CCS, COM



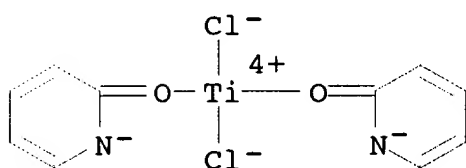
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
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 CI CCS



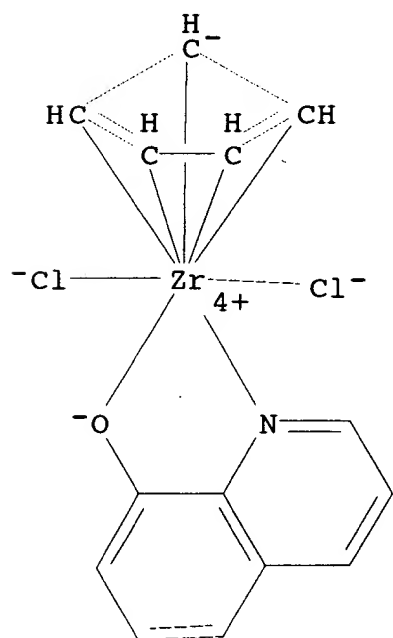




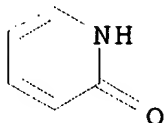
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN Titanium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI)  
 MF C10 H8 Cl2 N2 O2 Ti  
 CI CCS



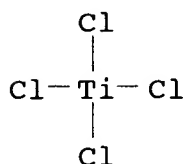
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
 MF C14 H11 Cl2 N O Zr  
 CI CCS



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
IN 2(1H)-Pyridinone (9CI)  
MF C5 H5 N O  
CI COM

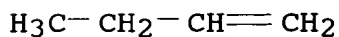


L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
IN Titanium chloride (TiCl<sub>4</sub>) (T-4)- (9CI)  
MF Cl<sub>4</sub> Ti  
CI COM

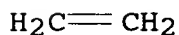


L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
IN 1-Butene, polymer with ethene (9CI)  
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
MF (C<sub>4</sub> H<sub>8</sub> . C<sub>2</sub> H<sub>4</sub>)<sub>x</sub>  
CI PMS

CM 1

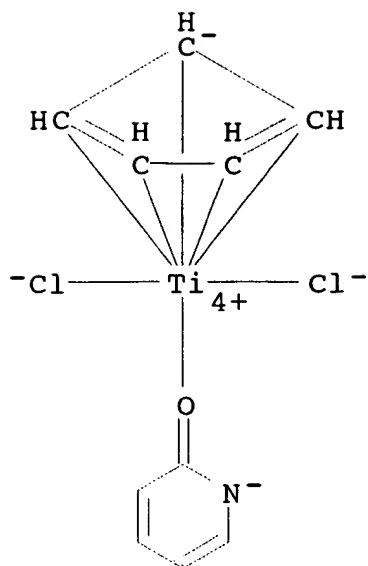


CM 2

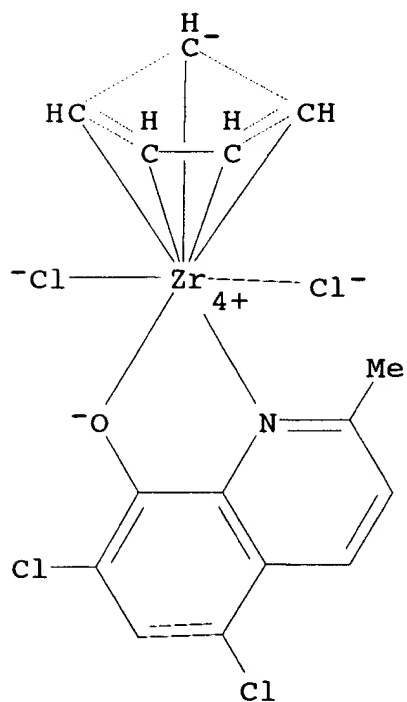


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
IN Titanium, dichloro(.eta.5-2,4-cyclopentadien-1-yl) (2(1H)-pyridinonato-.kappa.O2)- (9CI)  
MF Cl<sub>2</sub> H<sub>9</sub> Cl<sub>2</sub> N O Ti  
CI CCS

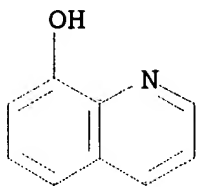


L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl) (5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8) - (9CI)  
 MF C15 H11 Cl4 N O Zr  
 CI CCS



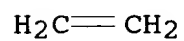
L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
 IN 8-Quinolinol (7CI, 8CI, 9CI)

MF C9 H7 N O  
CI COM



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS  
IN Ethene, homopolymer (9CI)  
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
MF (C2 H4)x  
CI PMS, COM

CM 1



ALL ANSWERS HAVE BEEN SCANNED

=> file reg

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STRUCTURE FILE UPDATES: 31 JUL 98 HIGHEST RN 209323-09-1  
DICTIONARY FILE UPDATES: 3 AUG 98 HIGHEST RN 209323-09-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 14, 1998

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Stereochemical name changes have been adopted and appear in CN's  
beginning 6/29/30. See the online news message for details.

=> d his

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DEL HIS Y  
ACT RAB659/A  
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L1 STR  
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L3 SCR 1838  
L4 SCR 1942  
L5 3550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4  
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L6 STR L1

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L7 50 S L6 SSS SAM SUB=L5

FILE 'HCAPLUS' ENTERED AT 13:33:38 ON 04 AUG 1998  
L8 0 S 126:31794/AN

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L9 1 S 1996:758983/AN  
SEL

L9 1 RN

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L10 14 S E1-E14  
L11 6 S L10 AND M/ELS AND N/ELS

FILE 'HCA' ENTERED AT 13:35:52 ON 04 AUG 1998  
L12 3 S L11

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L15 240 S L5 AND (TI OR ZR OR HF)/ELS

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L16 3028 S CAT# OR CATALY?  
L17 4444 S (POLYMER# OR HOMOPOLYMER# OR COPOLYMER# OR TERPOLYMER#  
L18 3571 S (POLYMERIZ? OR POLYMERIS? OR POLYM# OR CURE# OR CURING#  
L19 4525 S (POLYMER## OR HOMOPOLYMER## OR COPOLYMER## OR TERPOLYME

FILE 'HCA' ENTERED AT 13:46:37 ON 04 AUG 1998

L20 40131 S (POLYOLEFIN## OR OLEFIN##) (3A) (L18 OR L19)  
L21 1114 S L5  
L22 92 S L15  
L23 14303 S L20 AND L16  
L24 10 S L21 AND L23  
L25 18 S L22 AND L16  
L26 125753 S POLYOLEFIN## OR OLEFIN##  
L27 9 S L25 AND L26

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L28 126 S L6 AND L13 SSS FUL SUB=L5  
SAV L28 RAB659A/A

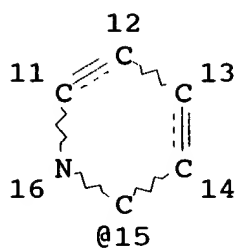
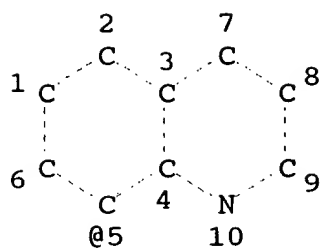
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L31 3 S L29 AND L20  
L32 3 S L29 AND L26  
L33 3 S L31 OR L32  
L34 5 S L12 OR L33  
L35 4 S L30 NOT L34  
L36 7 S (L24 OR L27) NOT (L34 OR L35)  
L37 52 S L29 NOT (L34 OR L35 OR L36)

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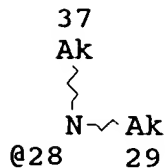
L1 STR



G1~~X~~G2~~X~~M~~~~~G3  
17 18 19 20

Ak @22

Cb @25



N~~~~~Ak  
@32 33

P~~~~~Ak  
@35 36

C~~X~~G4~~X~~N  
@38 39 @40

C~~X~~G4~~X~~O  
@43 44 @45

O~~~~~Ak  
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VAR G3=X/22/25/28/48  
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## GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 37

## STEREO ATTRIBUTES: NONE

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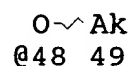
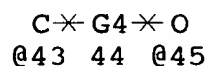
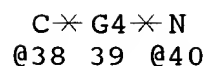
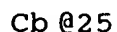
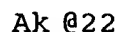
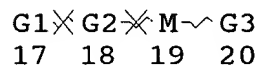
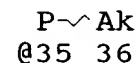
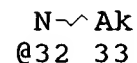
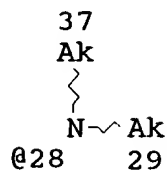
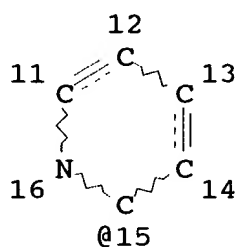
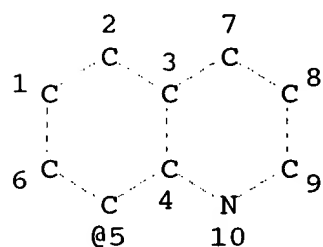
L4 SCR 1942

L5 3550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4

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L1 STR



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VAR G3=X/22/25/28/48

REP G4=(0-5) C



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## GRAPH ATTRIBUTES:

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## STEREO ATTRIBUTES: NONE

L2 SCR 1988 OR 1984 OR 2001 OR 1966 OR 1991 OR 1965  
L3 SCR 1838  
L4 SCR 1942  
L5 3550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4  
L15 240 SEA FILE=REGISTRY L5 AND (TI OR ZR OR HF)/ELS

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FILE COVERS 1967 - 1 Aug 1998 (980801/ED) VOL 129 ISS 6

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l34 1-5 cbib abs hitstr hitind

L34 ANSWER 1 OF 5 HCA COPYRIGHT 1998 ACS  
128:128339 Syndiotactic polymerization of styrene using  
titanium-8-hydroxyquinolate complex/methyl aluminoxane systems.  
Xu, Xuexiang; Zhou, Nai; Xie, Guanghua (Chinese Academy of Sciences,  
Institute of Chemistry, Beijing, 100080, Peop. Rep. China).

Gaofenzi Xuebao (6), 746-748 (Chinese) 1997. CODEN: GAXUE9. ISSN: 1000-3304. Publisher: Kexue Chubanshe.

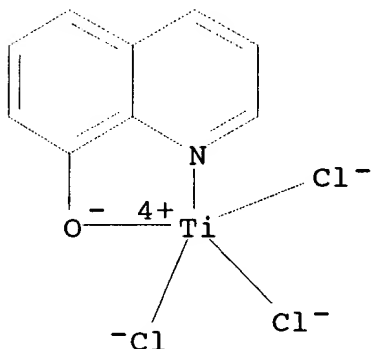
AB Titanium-8-hydroxyquinolate complexes in combination with Me aluminoxane (MAO) as cocatalyst are highly active towards styrene polymn., giving polymers with high syndiotacticity. The mol.-wt. distribution of polymers is broader, indicating the Ti complexes may be a "multi-site" catalyst.

IT 15614-57-0

(syndiotactic polymn. of styrene using titanium-8-hydroxyquinolate complex/methylaluminoxane systems as catalysts)

RN 15614-57-0 HCA

CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



CC 35-4 (Chemistry of Synthetic High Polymers)

IT 15614-57-0 16905-40-1 17442-90-9 17500-80-0

(syndiotactic polymn. of styrene using titanium-8-hydroxyquinolate complex/methylaluminoxane systems as catalysts)

L34 ANSWER 2 OF 5 HCA COPYRIGHT 1998 ACS

128:102528 Transition metal catalyst for the production of

**olefin polymers.** Reichle, Walter Thomas; Karol,

Frederick John (Union Carbide Chemicals + Plastics Technology Corp., USA). PCT Int. Appl. WO 9749713 A1 971231, 28 pp. DESIGNATED STATES: W: AU, BR, CA, JP, MX; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 97-US12236 970625. PRIORITY: US 96-670507 960627.

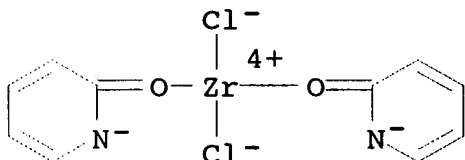
AB A catalyst compn. for the **polymn. of olefins**

comprises a bis(hydroxy arom. N ligand) transition metal catalyst precursor and an activating cocatalyst. A catalyst was prepd. by reaction of 2-hydroxypyridine (in PhMe) with n-BuLi (in hexane), then TiCl<sub>4</sub> to give a brown slurry (80 .mu.mole Ti/mL). This catalyst, activated with Me aluminoxane, was used to polyimd. C<sub>2</sub>H<sub>4</sub> at 65.degree. in 30 min.

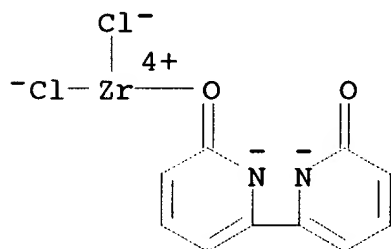
IT 201299-99-2 201300-00-7

(transition metal catalyst for prodn. of **ol fin****polym rs**)

RN 201299-99-2 HCA

CN Zirconium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI)  
(CA INDEX NAME)

RN 201300-00-7 HCA

CN Zirconium, [[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)-  
.kappa.O6]dichloro- (9CI) (CA INDEX NAME)

IC ICM C07F019-00

ICS C08F004-60; C08F004-602; C08F010-00

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

ST single site **polymn** catalyst **olefin**; transitionmetal **polymn** catalyst **olefin**; metallocene**polymn** catalyst **olefin**; hydroxy heteroarom

nitrogen bound metallocene catalyst; aluminoxane cocatalyst

metallocene catalyst **olefin polymn**

IT Methyl aluminoxanes

(cocatalyst; transition metal catalyst for prodn. of  
**olefin polymers**)

IT Polymerization catalysts

(hydroxypyridine bound transition metal; transition metal  
catalyst for prodn. of **olefin polymers**)

IT Metallocenes

(hydroxypyridine bound transition metal; transition metal  
catalyst for prodn. of **olefin polym rs**)IT 7550-45-0, Titanium tetrachloride, uses 10026-11-6, Zirconium  
tetrachloride 72762-00-6, 2-Hydroxypyridine **201299-99-2****201300-00-7**

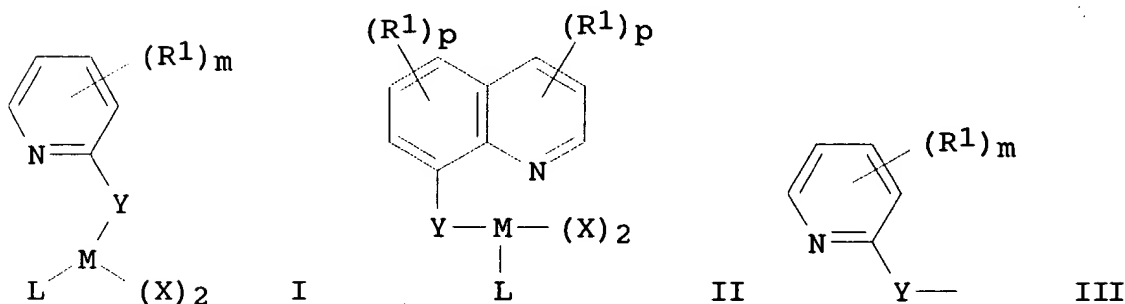
(transition metal catalyst for prodn. of **ol fin polymers**)

IT 9002-88-4P, Polyethylene 25213-02-9P, Ethylene-1-hexene copolymer  
(transition metal catalyst for prodn. of **olefin polymers**)

L34 ANSWER 3 OF 5 HCA COPYRIGHT 1998 ACS

126:31794 Transition metal catalysts based on bidentate ligands containing pyridine or quinoline moiety. Nagy, Sandor; Krishnamurti, Ramesh; Tyrell, John A.; Cribbs, Leonard V.; Cocoman, Mary (Occidental Chemical Corporation, USA). PCT Int. Appl. WO 9633202 A2 961024, 24 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 96-US3656 960318. PRIORITY: US 95-423232 950417.

GI



AB Transition metal catalysts for **.alpha.-olefin**

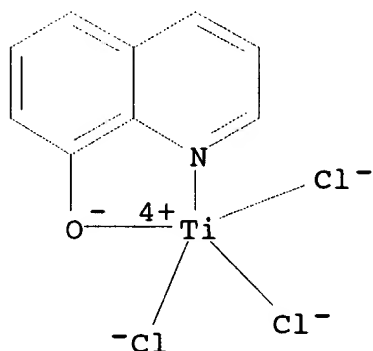
**polymn.** are characterized by having bidentate ligands contg. pyridine or quinoline moiety and have general structure I and II [Y = O, S, NR, (CR<sub>2</sub>)<sub>n</sub>NR, (CR<sub>2</sub>)<sub>n</sub>O; R = H, C1-6 alkyl; R' = R, C1-6 alkoxy, C6-16 aryl, halogen, CF<sub>3</sub>; M = Ti, Zr, Hf; X = halogen, C1-6 alkyl, C1-6 alkoxy, NR<sub>2</sub>; L = X, cyclopentadienyl, C1-6 alkyl-substituted cyclopentadienyl, indenyl, fluorenyl, III; m = 0-4; n = 1-4, p = 0-3]. Thus polyethylene with Mw/Mn 3.67 and melt flow rate 10.2 was produced by using a catalyst system including 8-quinolinoxytitanium trichloride, which was prepd. from 8-hydroxyquinoline and TiCl<sub>4</sub>, and Me aluminoxanes in a molar ratio of Al/Ti = 1074; the catalyst productivity was 167.9 kg/g Ti/h.

IT 15614-57-0P 184534-40-5P 184534-41-6P  
184534-42-7P 184534-43-8P 184534-44-9P

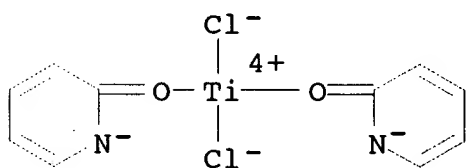
(transition metal catalysts based on bidentate ligands contg.

pyridine or quinoline moiety for .alpha.-olefin  
polymn.)

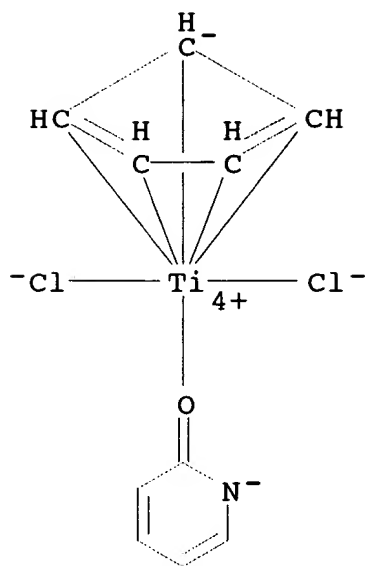
RN 15614-57-0 HCA  
CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA  
INDEX NAME)



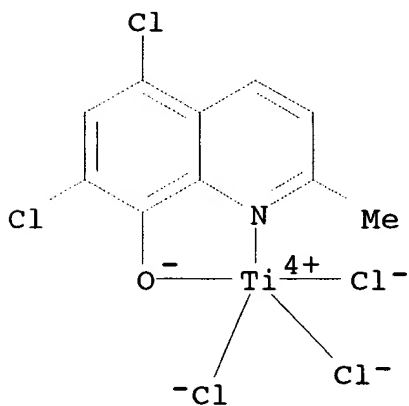
RN 184534-40-5 HCA  
CN Titanium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI)  
(CA INDEX NAME)



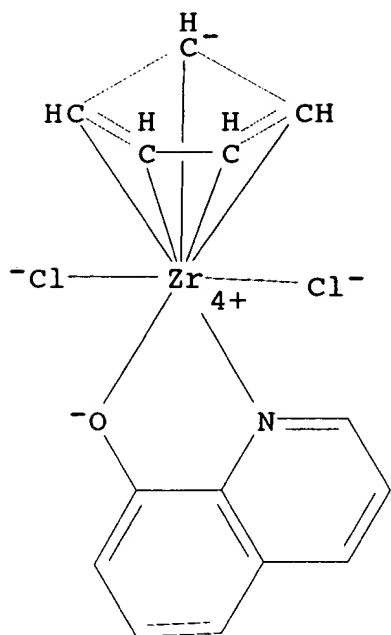
RN 184534-41-6 HCA  
CN Titanium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-  
pyridinonato-.kappa.O2)- (9CI) (CA INDEX NAME)



RN 184534-42-7 HCA  
 CN Titanium, trichloro(5,7-dichloro-2-methyl-8-quinolinolato-  
 .kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

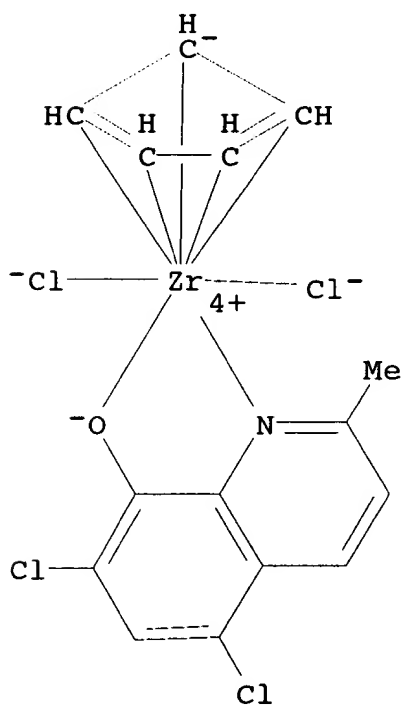


RN 184534-43-8 HCA  
 CN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-  
 .kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



RN 184534-44-9 HCA

CN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl) (5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



- IC ICM C07F017-00  
ICS B01J031-122; C08F010-00
- CC 35-3 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 29
- ST **polymn** catalyst **olefin** alpha; pyridine quinoline  
ligand transition metal catalyst
- IT Coordination polymerization catalysts  
(transition metal catalysts based on bidentate ligands contg.  
pyridine or quinoline moiety for **.alpha.-olefin**  
**polymn.**)
- IT Methyl aluminoxanes  
(transition metal catalysts based on bidentate ligands contg.  
pyridine or quinoline moiety for **.alpha.-olefin**  
**polymn.**)
- IT Linear low-density polyethylenes  
(transition metal catalysts based on bidentate ligands contg.  
pyridine or quinoline moiety for **.alpha.-olefin**  
**polymn.**)
- IT **15614-57-0P 184534-40-5P 184534-41-6P**  
**184534-42-7P 184534-43-8P 184534-44-9P**  
(transition metal catalysts based on bidentate ligands contg.  
pyridine or quinoline moiety for **.alpha.-olefin**  
**polymn.**)
- IT 9002-88-4P, Polyethylene 25087-34-7P  
(transition metal catalysts based on bidentate ligands contg.  
pyridine or quinoline moiety for **.alpha.-olefin**  
**polymn.**)
- L34 ANSWER 4 OF 5 HCA COPYRIGHT 1998 ACS
- 125:143539 **Olefin polymerization** catalyst and  
manufacture of **polyolefins** using the same with narrow  
molecular weight distribution. Nitto, Yu; Kaneshima, Tokitaka;  
Aoki, Toshiya (Asahi Kasei Kogyo Kabushiki Kaisha, Japan). PCT Int.  
Appl. WO 9618658 A1 960620, 164 pp. DESIGNATED STATES: W: CN, KR,  
US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT,  
SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 95-JP2558 951213.  
PRIORITY: JP 94-308729 941213; JP 94-308730 941213.
- AB An **olefin polymn.** catalyst contains a transition  
metal compd. composed of .gtoreq.1 transition metal selected from  
Ti, Zr and Hf and .gtoreq.2 ligands, one of which has a  
cyclopentadienyl skeleton and the other(s) of which is a monovalent  
bidentate anionic ligand contg. an element selected from O, S, Se  
and Te and one selected from N, S, Se and Te as coordinating atoms  
through which the ligand is coordinated with the transition metal,  
one of the latter ligands being optionally bonded to the group  
having a cyclopentadienyl skeleton through a crosslinking group; and  
a process for efficiently prepg. an **ol fin** homo- or  
**copolym r** with this catalyst. The **polymn.** of one or more  
**olefins** with the above catalyst can give a homopolymer  
having a narrow mol. wt. distribution or a copolymer having a narrow



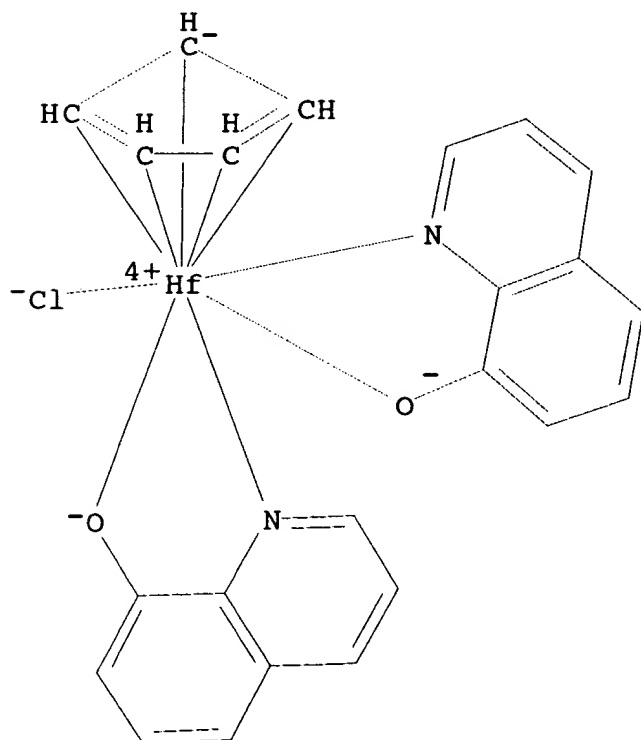
mol. wt. distribution and a uniform compn., and these homo- and copolymers are excellent in impact strength, stress cracking resistance, transparency, heat sealability at low temp. and blocking resistance and have low stickiness and extractible content. Ethylene was polymd. in the presence of methylaluminoxane and (pentamethylcyclopentadienyl)tris(dimethyldithiocarbamate)zirconium to give polyethylene with Mw 565,000 and Mw/Mn 2.56.

IT 33291-90-6P 180079-17-8P 180079-21-4P  
180079-22-5P 180079-23-6P 180079-29-2P  
180079-31-6P

(catalysts for polyolefins using the same with narrow mol. wt. distribution)

RN 33291-90-6 HCA

CN Hafnium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



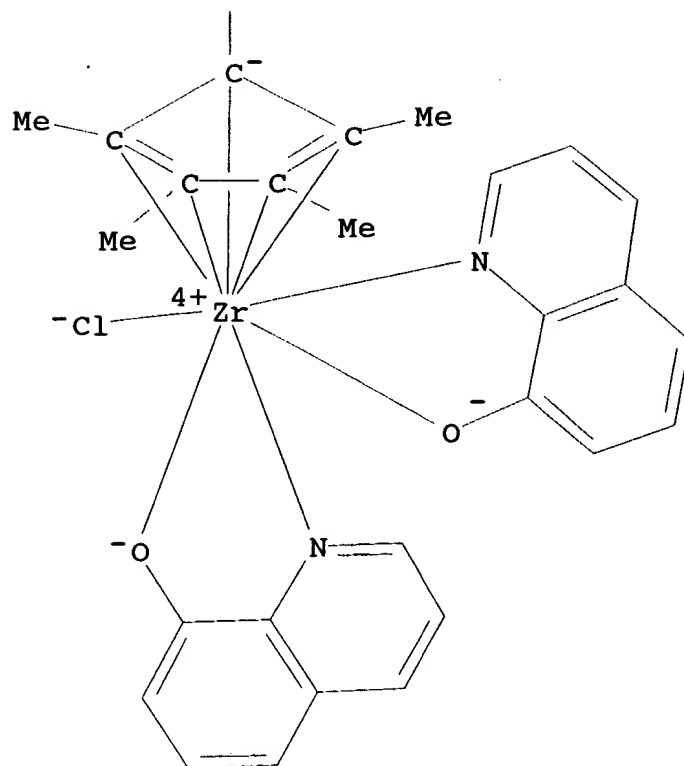
RN 180079-17-8 HCA

CN Zirconium, chloro[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

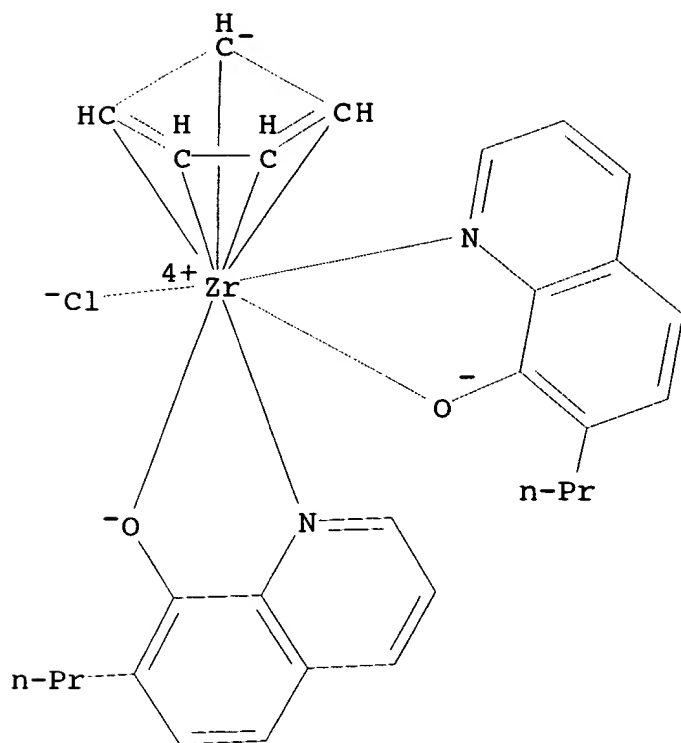
PAGE 1-A

Me  
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RN 180079-21-4 HCA  
CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(7-propyl-8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

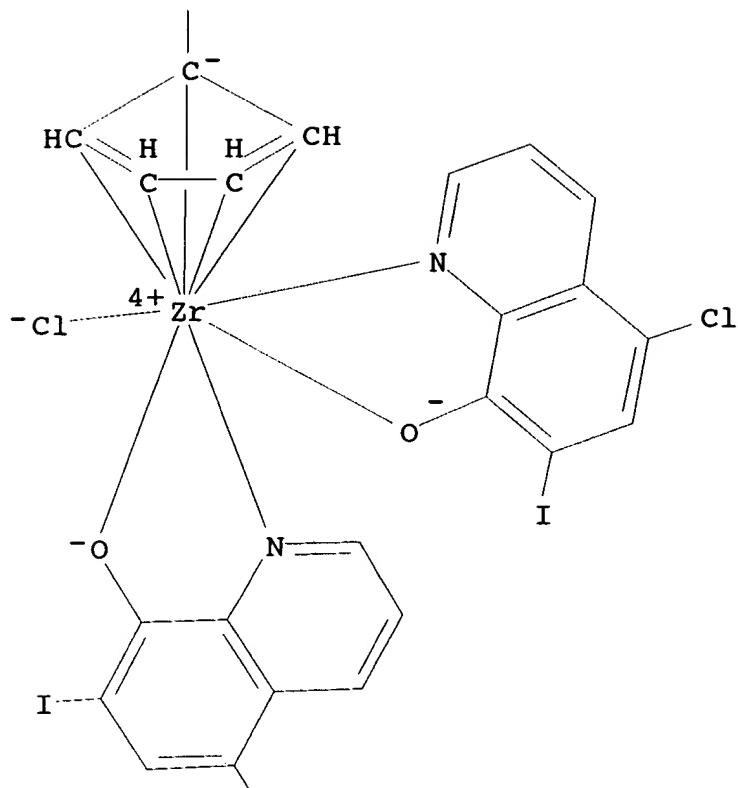


RN 180079-22-5 HCA  
 CN Zirconium, [(1,2,3,4,5-.eta.)-1-butyl-2,4-cyclopentadien-1-yl]chlorobis(5-chloro-7-iodo-8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

PAGE 1-A

n-Bu  
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PAGE 2-A



PAGE 3-A

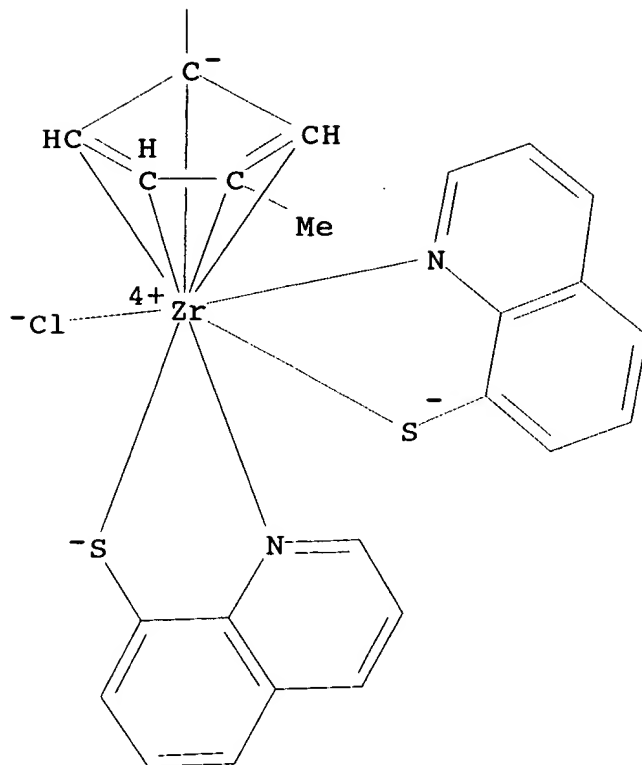
Cl

RN 180079-23-6 HCA  
 CN Zirconium, chloro[(1,2,3,4,5-eta.)-1,3-dimethyl-2,4-cyclopentadien-1-yl]bis(8-quinolinethiolato-N1,S8)- (9CI) (CA INDEX NAME)

PAGE 1-A

Me  
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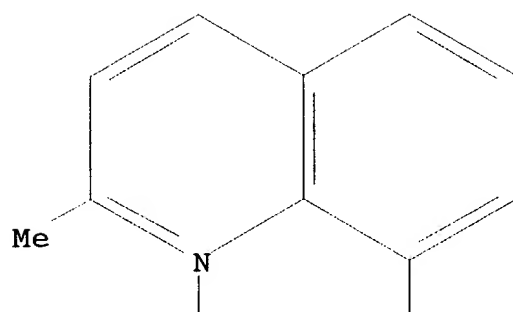
PAGE 2-A



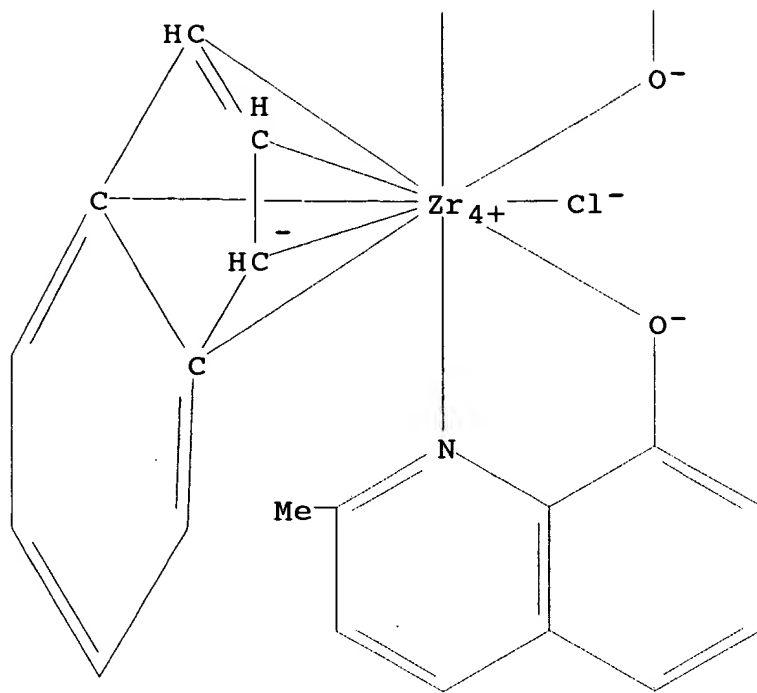
RN 180079-29-2 HCA  
CN Zirconium, chloro[(1,2,3,3a,7a-eta.)-1H-inden-1-yl]bis(2-methyl-8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



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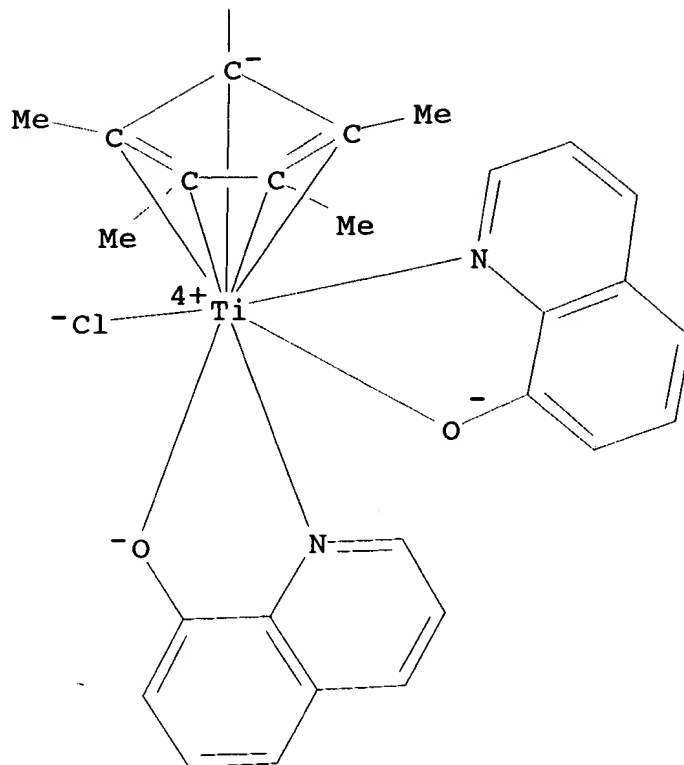


RN 180079-31-6 HCA  
 CN Titanium, chloro[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

PAGE 1-A

Me  
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PAGE 2-A



IC ICM C08F004-642  
 ICS C08F004-645; C08F010-00; C08F012-08; C08F032-00; C08F036-00  
 CC 35-3 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 67  
 ST transition metal complex **olefin polymn** catalyst;  
 ethylene hexene polymn catalyst; octene ethylene polymn catalyst  
 IT **Polymerization** catalysts  
 (olefin polymn. catalyst and manuf. of  
**polyolefins** using the same with narrow mol. wt.  
 distribution)  
 IT Alkenes  
 (polymers, olefin polymn. catalyst  
 and manuf. of **polyolefins** using the same with narrow  
 mol. wt. distribution)  
 IT 146355-12-6, Tris(pentafluorophenyl)borate  
 (catalysts for **polyolefins** using the same with narrow  
 mol. wt. distribution)  
 IT 33291-90-6P 65554-57-6P 66200-00-8P 74822-09-6P  
 110509-37-0P 137657-29-5P 180078-76-6P 180078-77-7P  
 180078-78-8P 180078-79-9P 180078-80-2P 180078-81-3P  
 180078-82-4P 180078-87-9P 180078-88-0P 180078-89-1P  
 180078-90-4P 180078-91-5P 180078-93-7P 180078-95-9P  
 180078-96-0P 180078-97-1P 180078-99-3P 180079-00-9P

180079-01-0P    180079-02-1P    180079-03-2P    180079-04-3P  
 180079-06-5P    180079-08-7P    180079-09-8P    180079-10-1P  
 180079-11-2P    180079-12-3P    180079-14-5P    180079-15-6P  
 180079-16-7P    **180079-17-8P**    180079-18-9P    180079-19-0P  
 180079-20-3P    **180079-21-4P**    **180079-22-5P**  
**180079-23-6P**    180079-24-7P    180079-25-8P    180079-26-9P  
 180079-27-0P    180079-28-1P    **180079-29-2P**    180079-30-5P  
**180079-31-6P**    180079-32-7P    180079-33-8P    180079-34-9P  
 180079-35-0P    180079-36-1P    180079-37-2P    180079-38-3P  
 180079-40-7P    180079-41-8P    180079-42-9P    180079-44-1P  
 180079-45-2P    180079-46-3P    180079-47-4P    180079-48-5P  
 (catalysts for **polyolefins** using the same with narrow  
 mol. wt. distribution)  
 IT    9002-88-4P, Polyethylene    25213-02-9P    26221-73-8P  
 (catalysts for **polyolefins** using the same with narrow  
 mol. wt. distribution)  
 IT    135181-14-5P    180078-84-6P  
 (catalysts for **polyolefins** using the same with narrow  
 mol. wt. distribution)  
 IT    75-77-4, Trimethylsilyl chloride, reactions    96-80-0,  
 2-Diisopropylaminoethanol    122-98-5, 2-Phenylaminoethanol  
 128-04-1, Sodium dimethyldithiocarbamate    130-16-5,  
 5-Chloro-8-quinolinol    130-26-7, 5-Chloro-7-iodo-8-quinolinol  
 140-89-6    140-90-9, Sodium O-ethylxanthate    141-33-3    148-24-3,  
 8-Quinolinol, reactions    491-33-8, 8-Quinolinethiol    555-24-8,  
 Phenoxyolithium    586-98-1, 2-Pyridinemethanol    643-62-9,  
 9-Acridinol    826-81-3, 2-Methyl-8-quinolinol    865-34-9,  
 Methoxyolithium    872-71-9    1068-22-0, Ammonium O,O'-  
 diethyldithiophosphate    1085-35-4    1271-19-8,  
 Bis(cyclopentadienyl)titanium dichloride    1470-61-7, Silver  
 diethyldithiocarbamate    2044-73-7, 2-Pyridinemethanethiol  
 2720-77-6    3743-22-4, 2-Dimethylaminophenol    4092-82-4, Sodium  
 diisopropyldithiocarbamate    4787-77-3, 2-Pyrrolidinophenol  
 12116-66-4, Bis(cyclopentadienyl)hafnium dichloride    12129-06-5,  
 (Pentamethylcyclopentadienyl)titanium trichloride    12148-49-1,  
 Bis(indenyl)zirconium dichloride    14159-57-0    18087-24-6,  
 2-Dimethylaminothiophenol    18938-33-5, Sodium  
 dibutyldiselenocarbamate    18992-87-5, Sodium dimethylthiocarbamate  
 23504-11-2    42508-74-7, 4-Methyl-2-pyridinemethanol    50742-62-6  
 54769-08-3    66542-75-4    67715-76-8    73364-10-0,  
 Bis(butylcyclopentadienyl)zirconium dichloride    75181-07-6,  
 (Pentamethylcyclopentadienyl)zirconium trichloride    81376-81-0  
 82387-86-8    102439-95-2    125542-03-2    180078-83-5    180078-85-7  
 180078-86-8    180078-92-6    180078-94-8    180078-98-2    180079-05-4  
 180079-07-6    180079-13-4    180079-39-4    180079-43-0  
 (catalysts for **polyolefins** using the same with narrow  
 mol. wt. distribution)

L34 ANSWER 5 OF 5 HCA COPYRIGHT 1998 ACS

68:39433 Reactions of 8-quinolinol with covalent halides. II. Tin(IV)  
 and titanium(IV) halides. Frazer, Malcolm J.; Rimmer, B. (Northern

Polytech., London, Engl.). J. Chem. Soc. A (1), 69-74 (English) 1968. CODEN: JCSIAP.

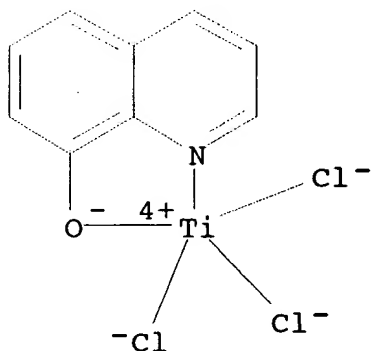
AB The adducts  $\text{MX}_4.2\text{OXH}$  ( $\text{M} = \text{Ti}$  or  $\text{Sn}$ ,  $\text{X} = \text{F}$ ,  $\text{Br}$ , and  $\text{I}$ ) are formed when 8-quinolinol ( $\text{OXH}$ ) (2 moles) in  $\text{CHCl}_3$  or tetrahydrofuran is added to the appropriate tetrahalide; with  $\text{M} = \text{Si}$  or  $\text{Ge}$ , however, adducts are not formed but there is loss of hydrogen halide and pptn. of the dihalodi-8-quinolinolato-metal  $\text{MX}_2\text{OX}_2$ . The 1:2 adducts, either by the action of heat ( $\text{X} = \text{F}$ ,  $\text{Br}$ , and  $\text{I}$ ), or by the addn. of excess of 8-quinolinol ( $\text{X} = \text{Br}$  and  $\text{I}$ ) give the corresponding  $\text{MX}_2\text{OX}_2$ . The dihalodi-8-quinolinolatotitanium compds. with excess 8-quinolinol give  $\text{TiXOX}_3$  in which  $\text{Ti}$  is probably heptacoordinate for  $\text{X} = \text{F}$  and  $\text{Br}$ . Iodotri-8-quinolinolatotitanium is a 1:1 electrolyte. The trichloro-8-quinolinolato-metals,  $\text{MCl}_3\text{OX}$  ( $\text{M} = \text{Ti}$  and  $\text{Sn}$ ), form adducts with 8-quinolinol and with pyridine, and probably contain a pentacoordinate metal atom.

IT 15614-57-0P

(prepn. of)

RN 15614-57-0 HCA

CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



CC 27 (Heterocyclic Compounds (One Hetero Atom))

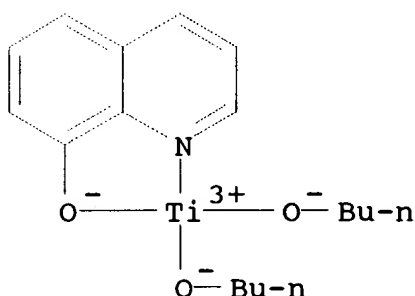
IT	15523-67-8P	15523-68-9P	<b>15614-57-0P</b>	16862-11-6P	
	16880-55-0P	16880-56-1P	16905-16-1P	16905-18-3P	16905-19-4P
	16905-20-7P	16905-21-8P	16905-22-9P	16905-23-0P	16905-24-1P
	16905-25-2P	16905-26-3P	16905-27-4P	16905-28-5P	16905-30-9P
	16905-31-0P	16905-32-1P	16905-33-2P	16905-34-3P	16905-35-4P
	16905-39-8P	16905-40-1P	16905-41-2P	16905-42-3P	16905-43-4P
	16905-44-5P	17211-42-6P	17211-44-8P	17211-45-9P	17211-46-0P
	17409-65-3P	18904-87-5P	20471-43-6P	20471-44-7P	20471-45-8P
	20471-46-9P	20471-47-0P	20471-48-1P	20471-49-2P	20471-50-5P
	21254-84-2P				

(prepn. of)

=> d l35 1-4 cbib abs hitstr hitind

L35 ANSWER 1 OF 4 HCA COPYRIGHT 1998 ACS

- 128:300202 **Catalytic** activity of titanium alkoxy derivatives in alcoholysis of ethoxysilanes. Khonina, T. G.; Kochneva, N. A.; Suvorov, A. L. (Ural Division, Institute of Organic Synthesis, Russian Academy of Sciences, Yekaterinburg, Russia). Russ. J. Gen. Chem., 67(1), 79-82 (English) 1997. CODEN: RJGCEK. ISSN: 1070-3632. Publisher: MAIK Nauka/Interperiodica Publishing.
- AB Titanium tetraalkoxides, regardless of their structure, are effective **catalysts** for alcoholysis of ethoxysilanes. Titanium alkoxychlorides demonstrate the highest **catalytic** activity, whereas the **catalytic** activity of coordination-satd. titanium compds. is the lowest. The influence of the **catalyst** nature on its activity is analyzed.
- IT 206053-84-1  
(**catalytic** activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)
- RN 206053-84-1 HCA
- CN Titanium, dibutoxy(8-quinolinolato-.kappa.N1,.kappa.O8)-, (T-4)-(9CI) (CA INDEX NAME)



- CC 67-2 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
- ST titanium alkoxy deriv **catalyst** alcoholysis ethoxysilane
- IT Alcoholysis **catalysts**  
Alcoholysis kinetics  
(**catalytic** activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)
- IT 546-68-9, Titanium tetraisopropoxide 1070-10-6 1790-25-6  
3087-36-3, Titanium tetraethoxide 3087-37-4, Titanium tetrapropoxide 3087-39-6, Titanium tetra-tert-butoxide 3112-68-3  
3374-12-7, Titanium tetra-sec-butoxide 4200-76-4 5593-70-4,  
Titanium tetrabutoxide 7393-49-9 7441-92-1 25902-23-2  
83328-25-0 206053-82-9 **206053-84-1**  
(**catalytic** activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)
- IT 78-07-9 78-10-4 78-62-6 2031-67-6  
(**catalytic** activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)
- IT 1591-02-2P 4766-57-8P 5581-68-0P 17957-38-9P  
(**catalytic** activity of titanium alkoxy derivs. in

## alcoholysis of ethoxysilanes)

L35 ANSWER 2 OF 4 HCA COPYRIGHT 1998 ACS

127:149211 Synthesis, Structures, Bonding, and Ethylene Reactivity of Group 4 Metal Alkyl Complexes Incorporating 8-Quinolinolato Ligands. Bei, Xiaohong; Swenson, Dale C.; Jordan, Richard F. (Department of Chemistry, University of Iowa, Iowa City, IA, 52242, USA). Organometallics, 16(15), 3282-3302 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical Society.

AB This contribution describes the synthesis, structures, bonding, and reactivity of neutral  $(Ox)_2MR_2$  and cationic  $(Ox)_2MR^+$  zirconium and hafnium alkyl complexes which contain substituted 8-quinolinolato ligands ( $Ox^- = 2-Me-8-quinolinolato$ ,  $MeOx^-$ , 2; 2-Me-5,7-Br2-8-quinolinolato,  $MeBr2Ox^-$ , 3). Alkane elimination and halide displacement reactions provide routes to  $(MeOx)_2ZrR_2$  (9a,  $R = CH_2Ph$ ; 9b,  $R = CH_2CMe_3$ ; 9c,  $R = CH_2SiMe_3$ ),  $(MeOx)_2Hf(CH_2Ph)_2$  (10a),  $(MeBr2Ox)_2ZrR_2$  (11a,  $R = CH_2Ph$ ; 11b,  $R = CH_2CMe_3$ ),  $(MeBr2Ox)_2Hf(CH_2Ph)_2$  (14a),  $(MeOx)_2ZrCl_2$  (15),  $(MeBr2Ox)_2ZrCl_2$  (16), and  $(MeBr2Ox)_2Zr(NMe_2)_2$  (17). The reaction of 16, 17, or  $(MeBr2Ox)_4Zr$  with  $AlMe_3$  yields  $(MeBr2Ox)AlMe_2$  (18). An x-ray crystallog. anal. shows that in the solid state 9a adopts a distorted octahedral structure with a trans-O, cis-N, cis-R ligand arrangement and that one of the benzyl ligands is bonded in an  $\eta^2$ -fashion. Soln. NMR data are consistent with this structure and establish that exchange of the distorted and normal benzyl ligands is rapid on the NMR time scale. Soln. NMR data for the other  $(Ox)_2MR_2$  complexes are consistent with analogous octahedral, trans-O, cis-N, cis-R structures for these species. Variable-temp. NMR studies establish that  $(Ox)_2MR_2$  complexes undergo inversion of metal configuration (i.e.,  $\Lambda/\Delta$  isomerization, racemization) on the NMR time scale at elevated temps. ( $\Delta G_{\text{thermod. (racemization)}} = 15-18 \text{ kcal/mol}$ ). Thermolysis of 11a results in migration of a benzyl ligand from Zr to C2 of a  $MeBr2Ox^-$  ligand, yielding  $(MeBr2Ox)(2-Me-2-CH_2Ph-5,7-Br2-Ox)ZrCH_2Ph$  (19) as a single diastereomer. Reaction of 9a or 9b with  $[HNMe_2Ph][B(C_6F_5)_4]$  yields the base-free cationic complexes  $[(MeOx)_2Zr(R)][B(C_6F_5)_4]$  (20a,  $R = CH_2Ph$ ; 20b,  $R = CH_2CMe_3$ ), while the corresponding reaction of 11a yields the labile amine adduct  $[(MeBr2Ox)_2Zr(CH_2Ph)(NMe_2Ph)][B(C_6F_5)_4]$  (21a). The reaction of  $[HNMePh_2][B(C_6F_5)_4]$  with the appropriate  $(Ox)_2M(CH_2Ph)_2$  complex yields 20a,  $[(MeOx)_2Hf(CH_2Ph)][B(C_6F_5)_4]$  (22a), or  $[(MeBr2Ox)_2M(CH_2Ph)][B(C_6F_5)_4]$  (23a,  $M = Zr$ ; 24a,  $M = Hf$ ). An x-ray crystallog. anal. establishes that the cation of 23a adopts a square pyramidal structure with a highly distorted ( $\eta^2$ ) benzyl ligand in the apical site and a trans-O, trans-N ligand arrangement in the basal sites, and NMR studies show that 23a and 24a adopt analogous structures in soln. In contrast, NMR studies establish that 20a, 20b, and 22a, which contain the more strongly electron-donating  $MeOx^-$  ancillary ligand, adopt distorted square pyramidal structures with an apical-O, cis-N ligand arrangement which allows max. O-M



.pi.-donation. The reactions of 23a or 24a with  $\text{PMe}_3$  yield the adducts  $[(\text{MeBr}_2\text{Ox})_2\text{M}(\text{CH}_2\text{Ph})(\text{PMe}_3)][\text{B}(\text{C}_6\text{F}_5)_4]$  (25a,  $\text{M} = \text{Zr}$ ; 26a,  $\text{M} = \text{Hf}$ ), which adopt trans-O, cis-N, cis-benzyl/ $\text{PMe}_3$  structures analogous to those of the  $(\text{Ox})_2\text{MX}_2$  complexes. The  $(\text{MeBr}_2\text{Ox})_2\text{M}(\eta^2\text{-CH}_2\text{Ph})^+$  cations 23a and 24a exhibit moderate ethylene polymn. activity, while the  $\text{MeOx}^-$  analogs 20a and 20b are inactive.

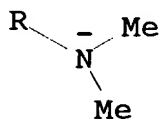
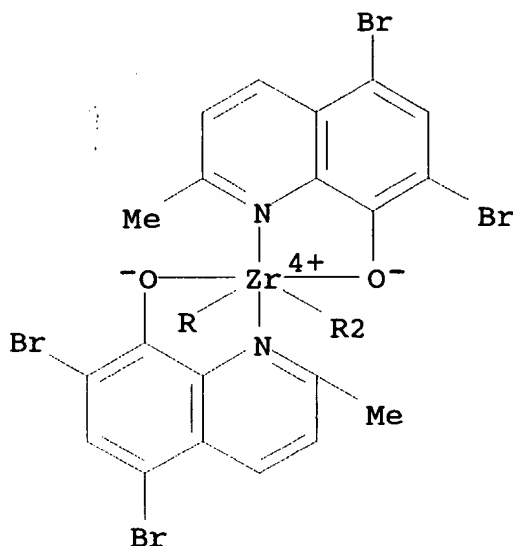
IT 193351-79-0P 193352-10-2P 193352-12-4P

(prepn. of)

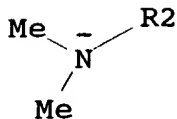
RN 193351-79-0 HCA

CN Zirconium, bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)bis(N-methylmethanaminato)-, (OC-6-13)- (9CI)  
(CA INDEX NAME)

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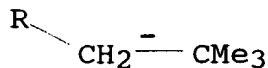
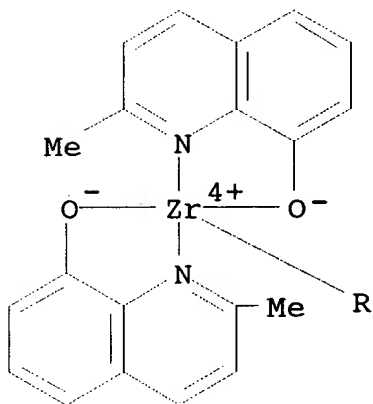
PAGE 2-A



RN 193352-10-2 HCA  
 CN Zirconium(1+), (2,2-dimethylpropyl)bis(2-methyl-8-quinolinolato-  
 .kappa.N1,.kappa.O8)-, (SP-5-31)-, tetrakis(pentafluorophenyl)borate  
 (1-) (9CI) (CA INDEX NAME)

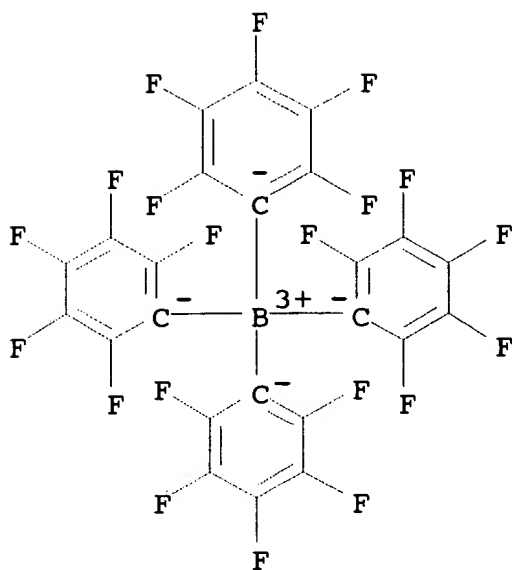
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CRN 193352-09-9  
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 CCI CCS  
 CDES 7:SP-5-31



CM 2

CRN 47855-94-7  
 CMF C24 B F20  
 CCI CCS

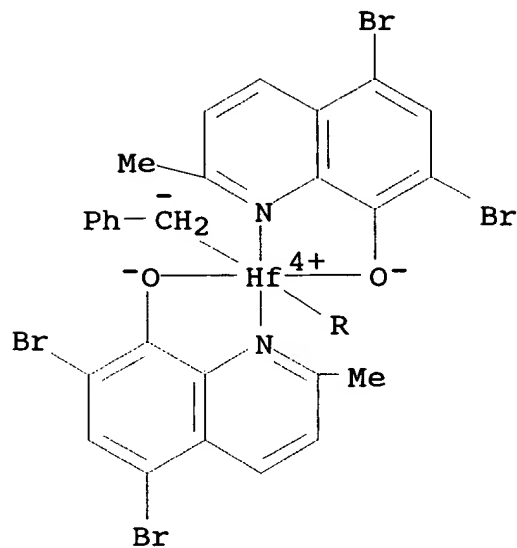


RN 193352-12-4 HCA  
 CN Hafnium(1+), bis(5,7-dibromo-2-methyl-8-quinolinolato-  
 .kappa.N1,.kappa.O8)(N,N-dimethylbenzenamine)(phenylmethyl)-,  
 (OC-6-13)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX  
 NAME)

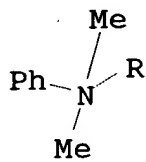
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 CMF C35 H30 Br4 Hf N3 O2  
 CCI CCS  
 CDES 7:OC-6-13

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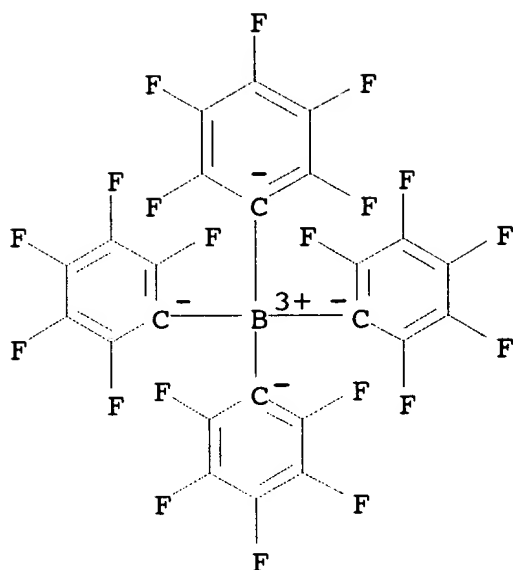


CM 2

CRN 47855-94-7

CMF C24 B F20

CCI CCS

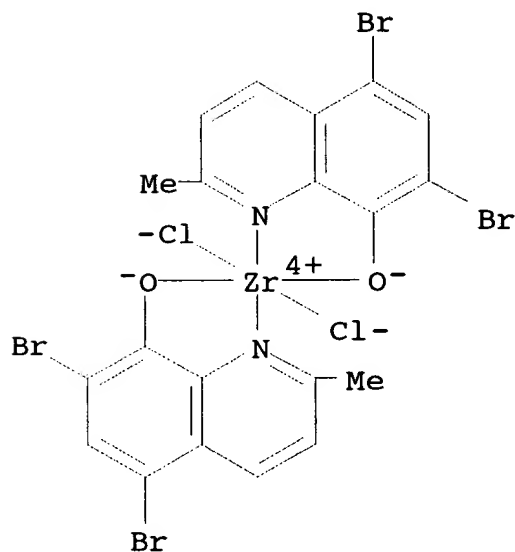


IT 193351-78-9P 193352-02-2P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-78-9 HCA

CN Zirconium, dichlorobis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-33)- (9CI) (CA INDEX NAME)

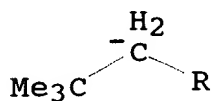
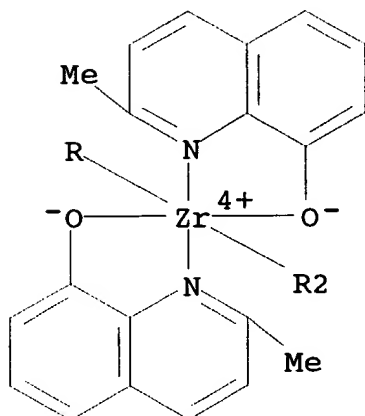


RN 193352-02-2 HCA

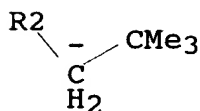
CN Zirconium, bis(2,2-dimethylpropyl)bis(2-methyl-8-quinolinolato-

.kappa.N1,.kappa.O8)-, (OC-6-13)- (9CI) (CA INDEX NAME)

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IT 193351-86-9P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-86-9 HCA

CN Zirconium(1+), bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8) (N,N-dimethylbenzenamine) (phenylmethyl)-, (OC-6-13)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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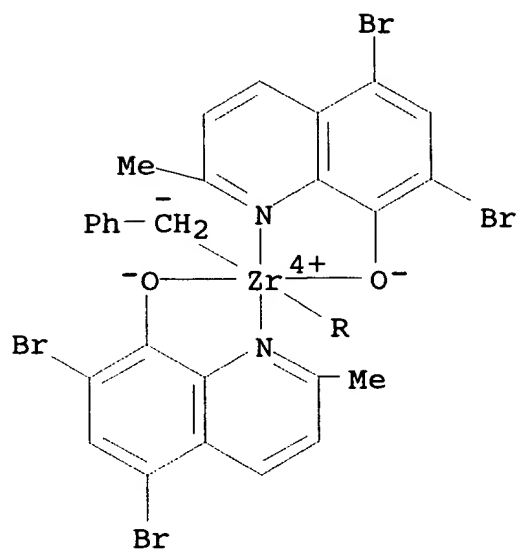
CRN 193351-85-8

CMF C35 H30 Br4 N3 O2 Zr

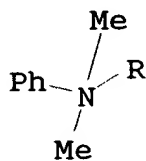
CCI CCS

CDES 7:OC-6-13

PAGE 1-A

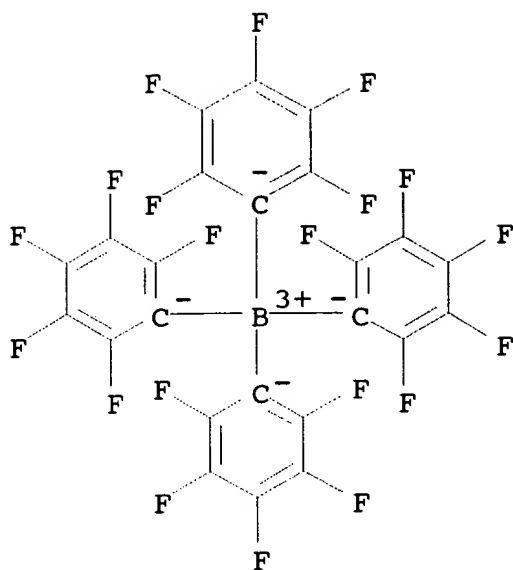


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CM 2

CRN 47855-94-7  
CMF C24 B F20  
CCI CCS

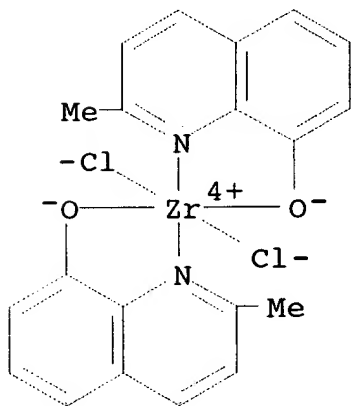


IT 193351-77-8P 193352-06-6P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-77-8 HCA

CN Zirconium, dichlorobis(2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-33)- (9CI) (CA INDEX NAME)

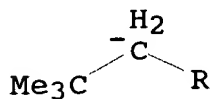
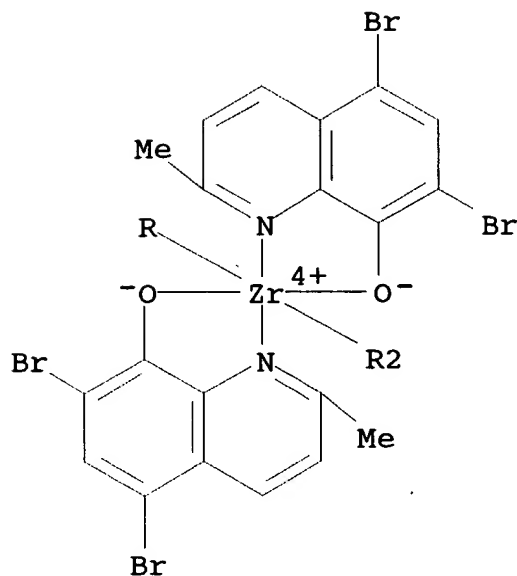


RN 193352-06-6 HCA

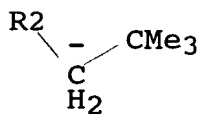
CN Zirconium, bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)bis(2,2-dimethylpropyl)-, (OC-6-13)- (9CI) (CA INDEX NAME)



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- CC 29-10 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 22, 35, 67, 75
- ST zirconium hafnium alkyl quinolinolato complex prepn; cationic  
 zirconium hafnium alkyl quinolinolato prepn; ethylene polymn  
**catalyst** quinolinolato zirconium hafnium; FMO quinolinolato  
 zirconium methyl complex; crystal structure benzylzirconium  
 quinolinolato cationic complex; mol structure benzylzirconium  
 quinolinolato cationic complex; isomerization kinetics  
 benzylzirconium benzylhafnium quinolinolato complex; racemization  
 kinetics zirconium hafnium quinolinolato alkyl
- IT Polymerization **catalysts**  
 (synthesis, structures, bonding, and ethylene polymn. activity of  
 Group 4 metal alkyl complexes incorporating quinolinolato  
 ligands)

- IT 9002-88-4P 193351-75-6P **193351-79-0P** 193351-80-3P  
193351-81-4P **193352-10-2P** **193352-12-4P**  
(prepn. of)  
IT **193351-78-9P** **193352-02-2P**  
(synthesis, structures, bonding, and ethylene polymn. activity of  
Group 4 metal alkyl complexes incorporating quinolinolato  
ligands)  
IT 193351-72-3P 193351-83-6P **193351-86-9P** 193351-89-2P  
193351-94-9P 193351-97-2P 193352-00-0P  
(synthesis, structures, bonding, and ethylene polymn. activity of  
Group 4 metal alkyl complexes incorporating quinolinolato  
ligands)  
IT 160883-74-9P 193351-70-1P **193351-77-8P** 193352-04-4P  
**193352-06-6P**  
(synthesis, structures, bonding, and ethylene polymn. activity of  
Group 4 metal alkyl complexes incorporating quinolinolato  
ligands)

L35 ANSWER 3 OF 4 HCA COPYRIGHT 1998 ACS

114:103008 **Catalysts** for the preparation of alternating  
polyesters from epoxides and cyclic anhydrides. Bagrel, Valerie;  
Garapon, Jacques; Touet, Remi; Huet, Catherine; Damin, Bernard  
(Institut Francais du Petrole, Fr.; Air Liquide, Societe Anon. pour  
l'Etude et l'Exploitation des Procedes Georges Claude; Elf France).  
Eur. Pat. Appl. EP 387119 A2 900912, 17 pp. DESIGNATED STATES: R:  
AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE. (French). CODEN:  
EPXXDW. APPLICATION: EP 90-400490 900221. PRIORITY: FR 89-3140  
890310.

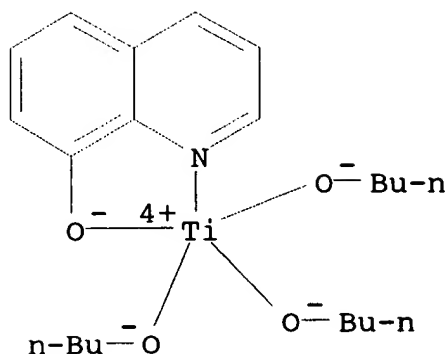
AB The Ti complexes  $Ti(OR_1)_m(OR_2)_n(OR_3)_pL_q$  ( $R_1-3$  = hydrocarbyl;  $L = N$   
compd.;  $m, n, p = 0$  or  $1$ ;  $Q = 1-4$ ;  $m + n + p + q = 4$ ) are  
**catalysts** for the alternating polymn. of epoxides with  
cyclic anhydrides. Stirring maleic anhydride 14.7, decycloxirane  
27.6,  $PhC_{12}H_{25}$  7.4,  $PhMe$  17.6, and tributoxy(8-quinolinato)titanium  
0.62 g at 100.degree. for 6 h gave a 95 and 90% conversion of  
epoxide and anhydride, resp., to a polyester with no.-av. mol. wt.  
7500, with little homopolymn. of the epoxide.

IT **14843-25-5**, Tributoxy(8-quinolinolato)titanium  
**131479-76-0**

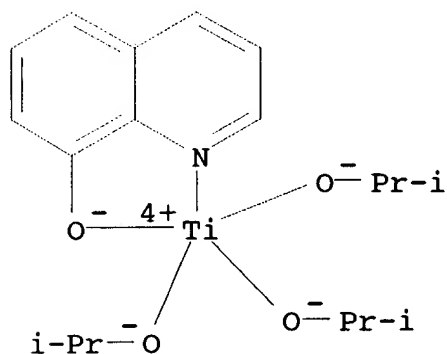
(**catalysts**, for alternating polymn. of epoxides with  
anhydrides)

RN 14843-25-5 HCA

CN Titanium, tributoxy(8-quinolinolato- $N_{1,08}$ )- (9CI) (CA INDEX NAME)



RN 131479-76-0 HCA  
 CN Titanium, tris(2-propanolato)(8-quinolinolato-N1,O8)- (9CI) (CA  
 INDEX NAME)



IC ICM C08G063-42  
 ICS C08G063-58  
 CC 35-3 (Chemistry of Synthetic High Polymers)  
 Section cross-reference(s): 67  
 ST **catalyst** polymn epoxide anhydride; titanium chelate  
**catalyst** polymn; quinolinol chelate titanium  
**catalyst**; polyester manuf epoxide anhydride; maleic  
 anhydride copolymer epoxide; decycloxirane copolymer anhydride  
 IT Polyesters, preparation  
 (manuf. of, by alternating polymn. of epoxides with cyclic  
 anhydrides, **catalysts** for)  
 IT Polymerization **catalysts**  
 (alternating, titanium nitrogen compd. complexes, for epoxides  
 with cyclic anhydrides)  
 IT Anhydrides  
 (cyclic, polymers, with epoxides, manuf. of, **catalysts**  
 for)  
 IT Epoxides  
 (polymers, with cyclic anhydrides, manuf. of, **catalysts**

for)

IT 14843-25-5, Tributoxy(8-quinolinolato)titanium 40506-24-9  
55235-58-0 131479-76-0 131479-77-1 132529-98-7

(**catalysts**, for alternatng polymn. of epoxides with  
anhydrides)

IT 131479-70-4P 131479-71-5P 131479-72-6P 131552-41-5P  
131552-44-8P 131552-50-6P  
(manuf. of, **catalysts** for)

L35 ANSWER 4 OF 4 HCA COPYRIGHT 1998 ACS

84:60078 Polymerization of butadiene on alkyl-o-titanate-  
triisobutylaluminum systems. Monakov, Yu. B.; Rafikov, S. R.;  
Ivanova, A. M.; Panasenko, A. A.; Tolstikov, G. A.; Pozdeeva, A. A.;  
Zaev, E. E.; Lukmanova, R. Z.; Igoshkina, G. S. (Bashk. Filial,  
Inst. Khim., Ufa, USSR). Vysokomol. Soedin., Ser. A, 17(12), 2631-6  
(Russian) 1975. CODEN: VYSAAF.

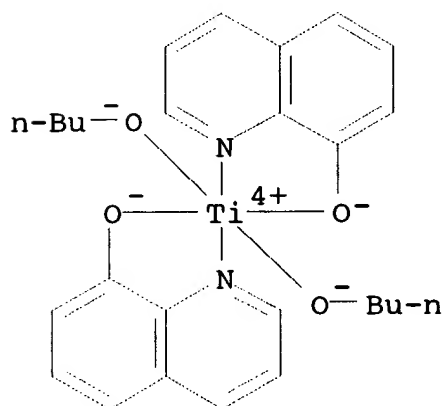
AB The polymn. of butadiene (I) in the presence of the binary  
**catalytic** system composed of triisobutylaluminum [100-99-2]  
and Ti(OR)<sub>4</sub> (where R = Bu-C<sub>9</sub>H<sub>19</sub>) at 22.degree. showed that the  
highest polymn. rate was reached in the presence of Ti(OBu)<sub>4</sub>  
[5593-70-4]-(iso-Bu)<sub>3</sub>Al at a ratio of Al:Ti = 8:1. The  
microstructure of polybutadiene [9003-17-2] was independent of  
monomer conversion or Al:Ti ratio. The ir spectra of the  
**catalytic** system contg. I suggest that the reactive polymn.  
sites are Ti(III) compds.

IT 17034-82-1

(**catalysts**, contg. triisobutylaluminum, for polymn. of  
butadiene)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 35-4 (Synthetic High Polymers)

ST butadiene polymn binary **catalyst**; titanium organo  
**catalyst** polymn; aluminum organo **catalyst** polymn;  
kinetics polymn butadiene **catalyst**

IT Polymerization **catalysts**  
(alkyl titanate-triisobutylaluminum, for butadiene)  
IT 100-99-2, uses and miscellaneous  
(**catalysts**, contg. alkyl titanates, for polymn. of  
butadiene)  
IT 1790-25-6 5593-70-4 6167-42-6 7360-52-3 10585-24-7  
16902-59-3 **17034-82-1** 22063-06-5  
(**catalysts**, contg. triisobutylaluminum, for polymn. of  
butadiene)  
IT 9003-17-2P  
(prepn. of, **catalysts** for)

=>

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L36 ANSWER 1 OF 7 HCA COPYRIGHT 1998 ACS

128:212149 A pyridine dialkoxide titanium dichloride complex. Synthesis and molecular structure of 2,6-bis(2,2-diphenyl-2-trimethylsilyloxyethyl)pyridine. Mack, Helmut; Eisen, Moris S. (Department of Chemistry, Technion-Israel Institute of Technology, Haifa, 32000, Israel). J. Chem. Soc., Dalton Trans. (6), 917-922 (English) 1998. CODEN: JCDBTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

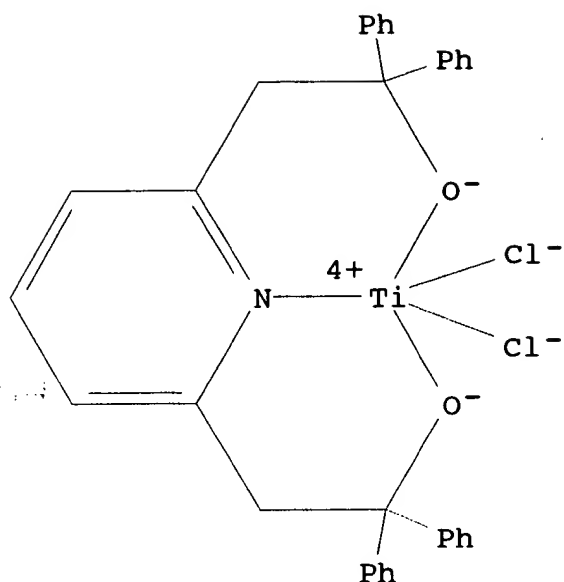
AB Reaction of 2,6-dimethylpyridine with 2 equiv of LiBu followed by addn. of 2 equiv of benzophenone and the consecutive reaction with 2 equiv of SiMe3Cl afforded the doubly functionalized 2,6-bis(2,2-diphenyl-2-trimethylsilyloxyethyl)pyridine L. The structure of L was detd. by an x-ray diffraction study. Reaction of either a doubly lithiated intermediate or the corresponding silylated ligand L with TiCl4 afforded a pyridine dialkoxide titanium dichloride complex TiL'Cl2 (LH2 = 2,6-pyridinebis(2,2-diphenylethan-2-ol)). A cationic .alpha.-olefin **polymn. catalyst** was generated from this complex with an excess of methylaluminoxane (MeAlO)n. A comparison of the **catalytic** activity with those of similar bis(alkoxide) complexes is presented.

IT 203986-89-4P

(prepn. and **catalytic** activity in .alpha.-  
**olefin polymn.** with methylaluminoxane)

RN 203986-89-4 HCA

CN Titanium, dichloro[.alpha.,.alpha.,.alpha.',.alpha.'-tetraphenyl-2,6-pyridinediethanolato(2-)-.kappa.N1,.kappa.O2,.kappa.O6]-, (TB-5-22)-(9CI) (CA INDEX NAME)



- CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 27, 67, 75
- ST crystal structure bisdiphenylsilyloxyethylpyridine;  
 silyloxydiphenylethylpyridine prepn structure reaction titanium;  
 titanium pyridinebis(diphenylethanolato) complex prepn  
**catalyst; olefin polymn titanium**  
 pyridinebis(diphenylethanolato) complex **catalyst**
- IT Methyl aluminoxanes  
 (**catalytic** activity in .alpha.-olefin  
**polymn.** with titanium pyridinebis(diphenylethanolato)  
 chloro complex)
- IT .alpha.-Alkenes  
 (**catalytic** polymn. by titanium  
 pyridinebis(diphenylethanolato) chloro complex)
- IT Coordination polymerization **catalysts**  
 Polymerization  
 (**catalytic** **polymn.** of .alpha.-olefins  
 by titanium pyridinebis(diphenylethanolato) chloro complex)
- IT 74-85-1, Ethylene, reactions 115-07-1, Propene, reactions  
 (**catalytic** **polymn.** by titanium  
 pyridinebis(diphenylethanolato) chloro complex)
- IT 9002-88-4P, Polyethylene 9003-07-0P, Polypropylene  
 (**catalytic** **polymn.** of .alpha.-olefins  
 by titanium pyridinebis(diphenylethanolato) chloro complex)
- IT 203986-89-4P  
 (prepn. and **catalytic** activity in .alpha.-  
**ol fin polymn.** with methylaluminoxane)

**Bidentate Pyridine-Alkoxide Ligands. Synthesis and Polymerization Chemistry of (pyCR2O)2Zr(CH2Ph)2 and**

(pyCR2O)2Zr(CH2Ph)+ Complexes. Tsukahara, Toru; Swenson, Dale C.; Jordan, Richard F. (Department of Chemistry, University of Iowa, Iowa City, IA, 52242, USA). Organometallics, 16(15), 3303-3313 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical Society.

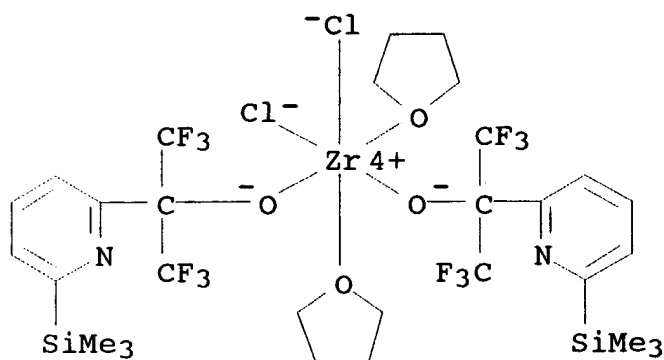
- AB The reaction of Zr(CH2Ph)4 with the pyridine alcs. 6-pyCR1R2OH (2a, R1 = R2 = CF3; 2b, R1 = R2 = Me; 2c, R1 = H, R2 = CF3) yields dibenzyl complexes (pyCR1R2O)2Zr(CH2Ph)2 (3a-c). These species adopt distorted octahedral structures with a trans-O, cis-N, cis-C ligand arrangement but undergo rapid inversion of configuration at Zr on the NMR time scale, with racemization barriers in the range from 8.6 (3b) to 10.1 (3c) kcal/mol. 3A and 3b react with B(C6F5)3 to yield [(pyCR1R2O)2Zr(CH2Ph)][PhCH2B(C6F5)3] (6a,b) and with [HNMe2Ph][B(C6F5)4] to yield [(pyCR1R2O)2Zr(CH2Ph)][B(C6F5)4] (7a,b). NMR spectra indicate that 6a,b and 7a,b are not strongly ion-paired in CD2Cl2. 6A polymerizes ethylene and 1-hexene to low mol. wt. polymers. [{PyCH(CF3)O}2Zr(CH2Ph)][PhCH2B(C6F5)3] (6c, generated in situ) is much less active for ethylene polymn. than 6a, and 6b is inactive.

IT 192432-42-1P

(prepn. and thermal loss of THF from)

RN 192432-42-1 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis(trifluoromethyl)-6-(trimethylsilyl)-2-pyridinemethanolato-.kappa.O2]dichlorobis(tetrahydrofuran)- (9CI) (CA INDEX NAME)

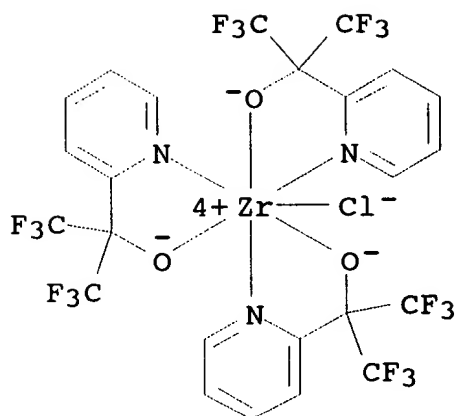


IT 192432-41-0P 192432-43-2P

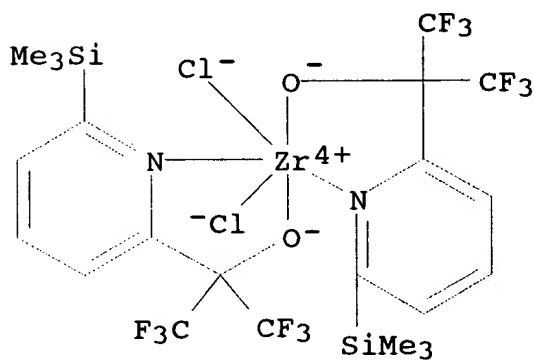
(prepn. of)

RN 192432-41-0 HCA

CN Zirconium, tris[.alpha.,.alpha.-bis(trifluoromethyl)-2-pyridinemethanolato-.kappa.N1,.kappa.O2]chloro- (9CI) (CA INDEX NAME)



RN 192432-43-2 HCA  
 CN Zirconium, bis[.alpha.,.alpha.-bis(trifluoromethyl)-6-(trimethylsilyl)-2-pyridinemethanolato-.kappa.N1,.kappa.O2]dichloro-, (OC-6-13)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 35, 75  
 ST **olefin polymn catalyst** zirconium  
 benzyl pyridinealkoxo; zirconium benzyl pyridinealkoxo prepn  
 structure **catalysis**; crystal structure zirconium benzyl  
 pyridinealkoxo complex; mol structure zirconium benzyl  
 pyridinealkoxo complex; racemization barrier zirconium benzyl  
 pyridinealkoxo  
 IT **Polyolefins**  
 (prepn. **catalyzed** by zirconium benzyl pyridinealkoxo  
 complexes)  
 IT Alcohols, preparation  
 (pyridinealkoxides, zirconium benzyl complexes; prepn., crystal  
 structure and **catalysis** of **olefin**  
**polymn.** by)  
 IT Methyl aluminoxanes  
 (zirconium benzyl pyridinealkoxo complex and MAO as



- catalyst for ol fin polymn.)**
- IT Polymerization **catalysts**  
(zirconium benzyl pyridinealkoxo complexes for **olefins**)
- IT 50981-41-4P, Polyhexene  
(atactic; zirconium benzyl pyridinealkoxo complex as  
**catalyst** for prepn. of low mol. wt.)
- IT 136040-19-2, Triphenylmethylium tetrakis(pentafluorophenyl)borate(1-  
)  
(for prepn. of **olefin polymn.**  
**catalyst** from zirconium benzyl pyridinealkoxo complexes)
- IT 1109-15-5, Tris(pentafluorophenyl)borane 118612-00-3,  
Dimethyl(phenyl)ammonium tetrakis(pentafluorophenyl)borate  
(for prepn. of **olefin polymn.**  
**catalysts** from zirconium benzyl pyridinealkoxo complexes)
- IT 192432-50-1  
(in situ formation and **catalysis** of **olefin**  
**polymn.** by)
- IT 192432-47-6P 192525-61-4P  
(prepn. and **catalysis** of **olefin**  
**polymn.**)
- IT 192432-42-1P  
(prepn. and thermal loss of THF from)
- IT 192432-37-4P 192432-41-0P 192432-43-2P  
192432-48-7P 192432-51-2P 192432-52-3P 192525-63-6P  
192525-64-7P  
(prepn. of)
- IT 192432-45-4 192525-62-5  
(prepn., fluxionality and **catalysis** of **olefin**  
**polymn.**)
- IT 192432-38-5P  
(prepn., soln. racemization, **catalysis** of  
**olefin polymn.** with MAO and reactions with  
triarylboron or tetraarylborate)
- IT 9002-88-4P, Polyethylene  
(zirconium benzyl pyridinealkoxo complexes as **catalysts**  
for prepn. of low mol. wt.)

L36 ANSWER 3 OF 7 HCA COPYRIGHT 1998 ACS

127:75019 Synthesis, Structures, Dynamics, and **Olefin**

**Polymerization** Behavior of Group 4 Metal (pyCar2O)2M(NR2)2

Complexes Containing Bidentate Pyridine-Alkoxide Ancillary Ligands.  
Kim, Il; Nishihara, Yasushi; Jordan, Richard F.; Rogers, Robin D.;  
Rheingold, Arnold L.; Yap, Glenn P. A. (Department of Chemistry,  
University of Iowa, Iowa City, IA, 52242, USA). Organometallics,  
16(15), 3314-3323 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333.  
OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical  
Society.

AB The reaction of 2-lithiopyridine and the appropriate diarylketone  
followed by hydrolysis yields pyCar2OH pyridine-alcs. (1a, Ar =  
4-tBu-C6H4; 1b, pyCar2OH = 2-pyridyl-9-fluorenyl; 1c, Ar =  
3-CF3-C6H4; 1d, Ar = 4-Ph-C6H4; 1e, Ar = 4-NEt2-C6H4; 1f, pyCar2OH =

1-(2-pyridyl)-1-dibenzosuberol; 1g, Ar = 3,5-(CF<sub>3</sub>)<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>). The reaction of Ti(NMe<sub>2</sub>)<sub>4</sub> with 2 equiv of 1a-g yields (pyCAR2O)<sub>2</sub>Ti(NMe<sub>2</sub>)<sub>2</sub> (2a-g) and NMe<sub>2</sub>H. The reaction of Zr(NMe<sub>2</sub>)<sub>4</sub> with 2 equiv of 1a,b,e yields (pyCAR2O)<sub>2</sub>Zr(NMe<sub>2</sub>)<sub>2</sub> (3a,b,e), while similar reactions with 1c,d yield mixts. of (pyCAR2O)<sub>x</sub>Zr(NMe<sub>2</sub>)<sub>4-x</sub> (x = 1-3) species. {PyC(3-CF<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>O}<sub>3</sub>Zr(NMe<sub>2</sub>) (4c) and {pyC(4-NEt<sub>2</sub>-C<sub>6</sub>H<sub>4</sub>)<sub>2</sub>O}<sub>4</sub>Zr (5e) were prep'd. from Zr(NMe<sub>2</sub>)<sub>4</sub> and 3 equiv of 1c or 4 equiv of 1e, resp. The reaction of Hf(NMe<sub>2</sub>)<sub>4</sub> with 2 equiv of 1a,e yields (pyCAR2O)<sub>2</sub>Hf(NMe<sub>2</sub>)<sub>2</sub> (6a,e), while reaction with 3 equiv of 1b,c yields (pyCAR2O)<sub>3</sub>Hf(NMe<sub>2</sub>) (7b,c). X-ray crystallog. analyses establish that 2b, 2e.cntdot.toluene, and 3a.cntdot.0.5NMe<sub>2</sub>H adopt distorted octahedral structures with a trans-O, cis-py, cis-amide arrangement of ligands. NMR data show that (pyCAR2O)<sub>2</sub>M(NMe<sub>2</sub>)<sub>2</sub> complexes adopt the same structure in soln. but undergo inversion of configuration at the metal with racemization barriers (.DELTA.G.thermod. (racemization)) at 12-14 kcal/mol. Treatment of (pyCAR2O)<sub>2</sub>M(NMe<sub>2</sub>)<sub>2</sub> complexes with Al(iBu)<sub>3</sub> and methylalumoxane (MAO) yields active, multisite ethylene polymn.

**catalysts.**

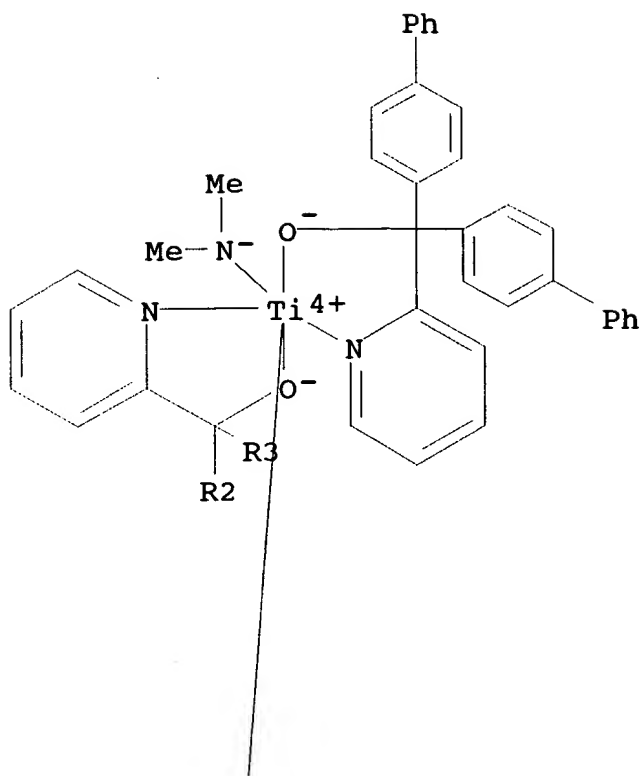
IT 191334-13-1P 191334-25-5P

(prepn. and catalyst for polymn. of ethylene)

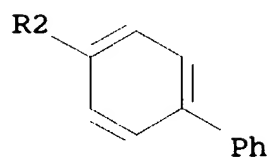
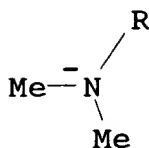
RN 191334-13-1 HCA

CN Titanium, bis[.alpha.,.alpha.-bis([1,1'-biphenyl]-4-yl)-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

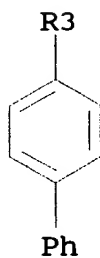
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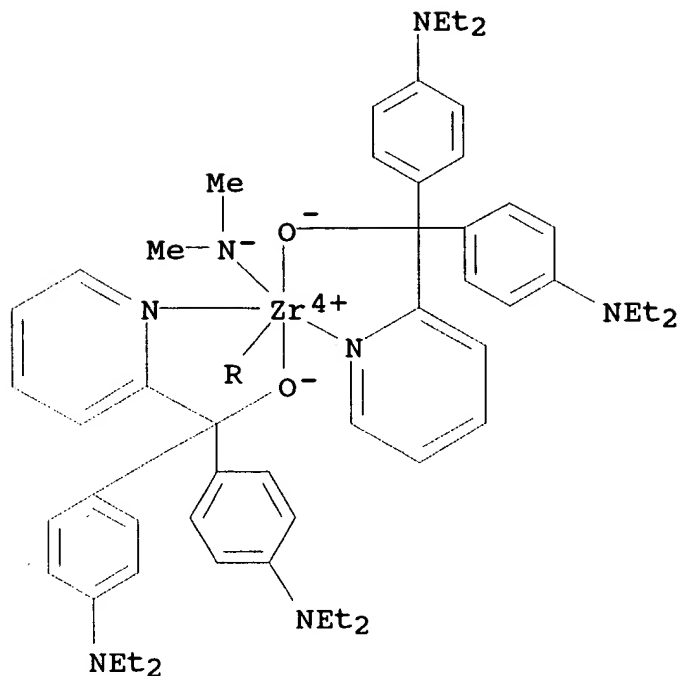


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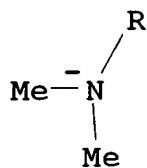


RN 191334-25-5 HCA  
CN Zirconium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

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IT 191334-39-1P 191334-41-5P

(prepn. and crystal structure)

RN 191334-39-1 HCA

CN Titanium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)-, compd. with methylbenzene (1:1) (9CI) (CA INDEX NAME)

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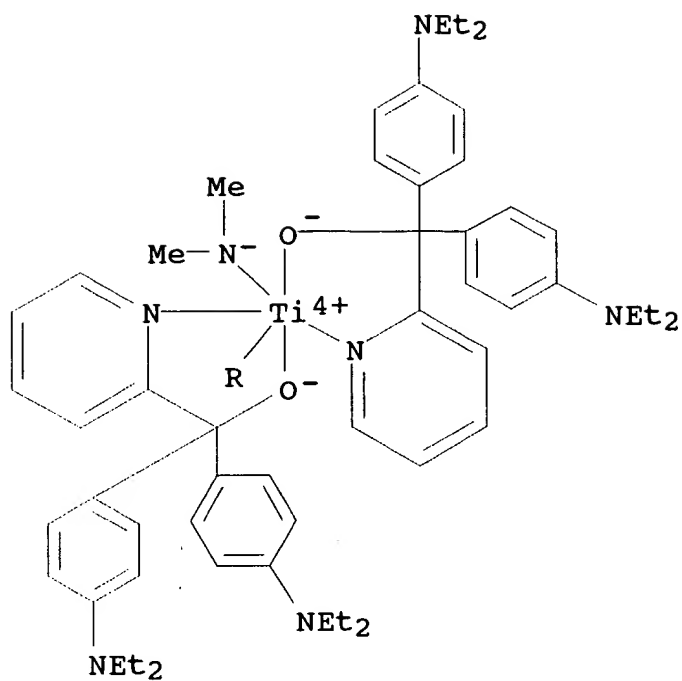
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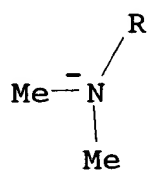
CCI CCS

CDES 7:OC-6-13

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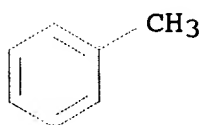
PAGE 2-A



CM 2

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CMF C7 H8

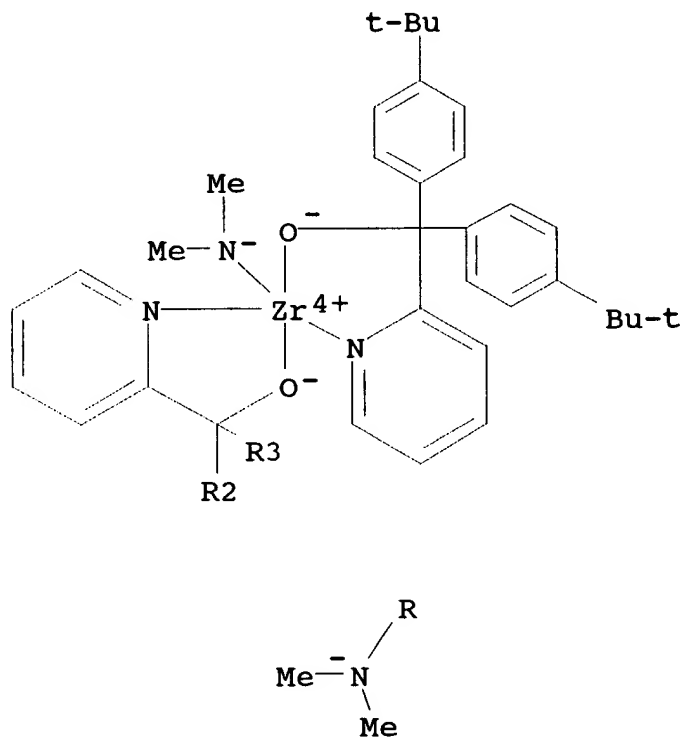


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CN Zirconium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)-, compd. with N-methylmethanamine (2:1) (9CI) (CA INDEX NAME)

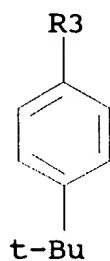
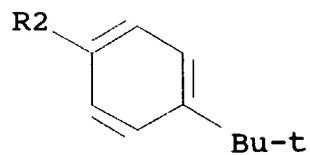
CM 1

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CMF C56 H72 N4 O2 Zr  
CCI CCS  
CDES 7:OC-6-13

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CM 2

CRN 124-40-3

CMF C2 H7 N



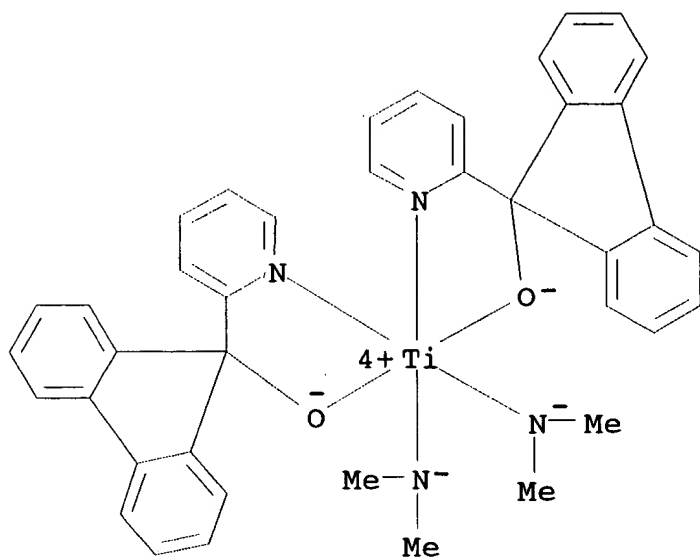
IT 191334-09-5P

(prepn. and crystal structure and **catalyst** for polymn.  
of ethylene)

RN 191334-09-5 HCA

CN Titanium, bis(N-methylmethanaminato)bis[9-(2-pyridinyl-.kappa.N)-9H-fluoren-9-olato-.kappa.O]-, (OC-6-13)- (9CI) (CA INDEX NAME)





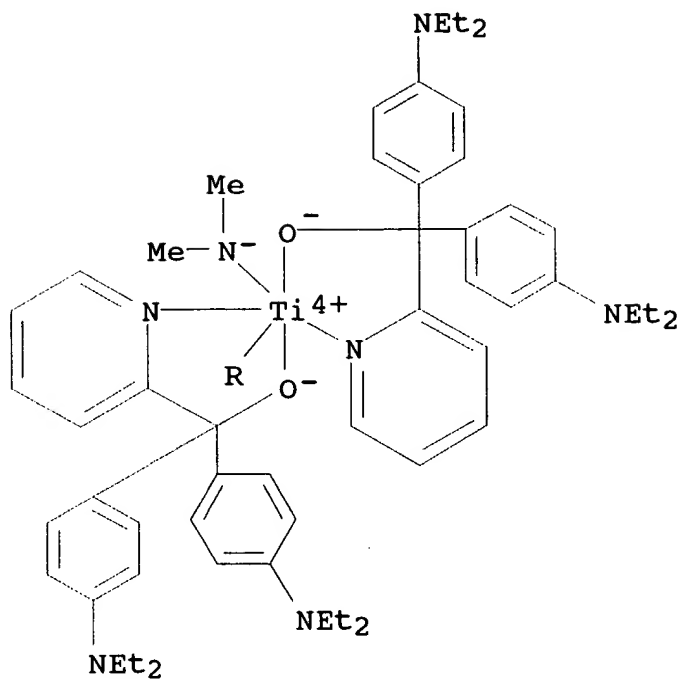
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(prepn. and mol. structure and catalyst for polymn. of ethylene)

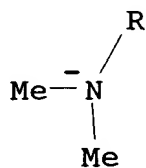
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CN Titanium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

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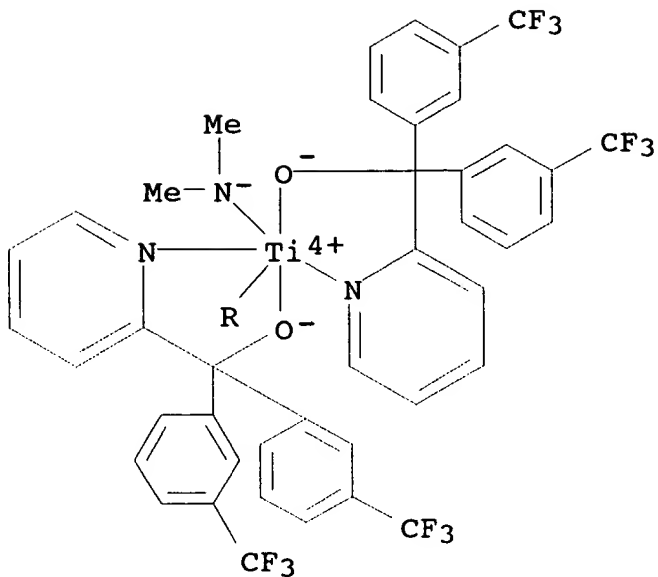
IT 191334-11-9P 191334-17-5P 191334-19-7P  
 191334-31-3P 191334-33-5P

(prepn. and racemization barrier)

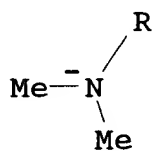
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CN Titanium, bis[.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

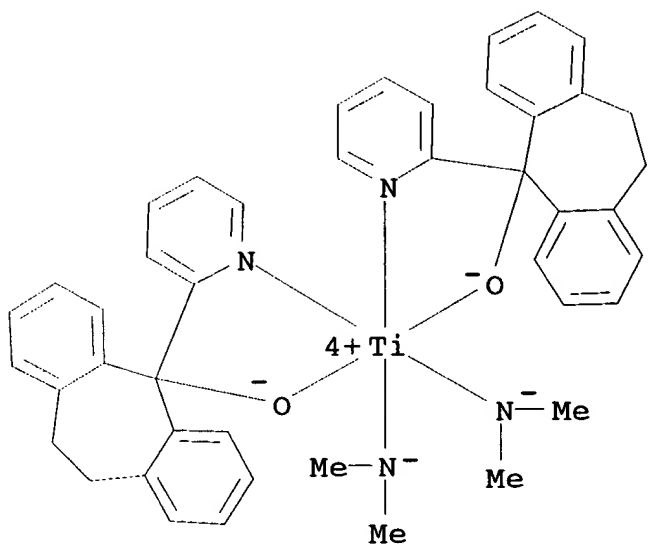
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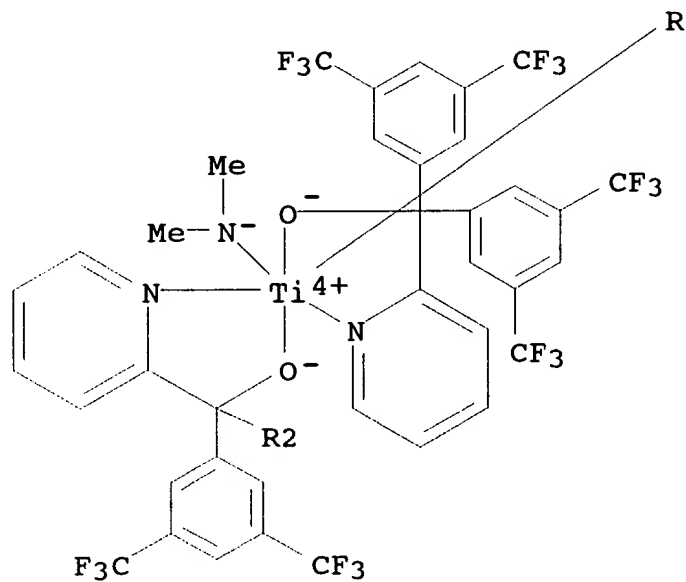


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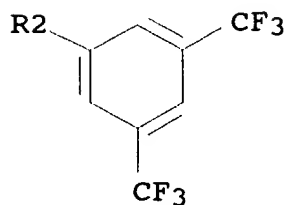
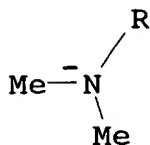


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 CN Titanium, bis[.alpha.,.alpha.-bis[3,5-bis(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

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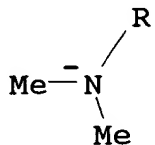
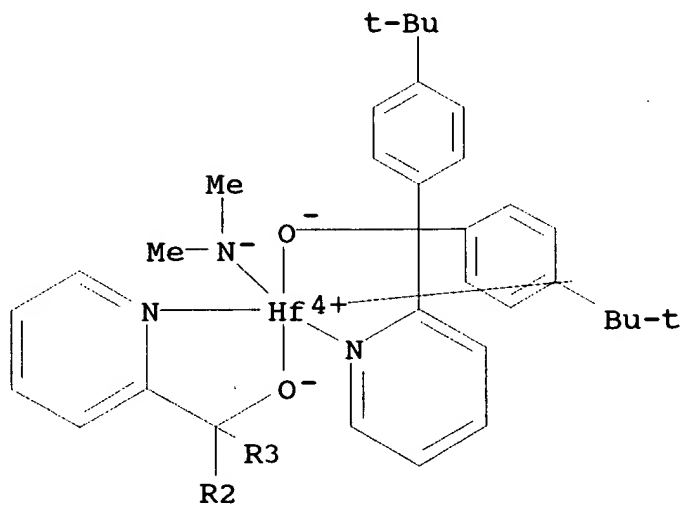


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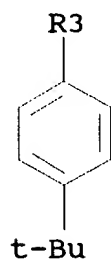
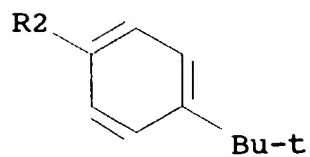


RN 191334-31-3 HCA  
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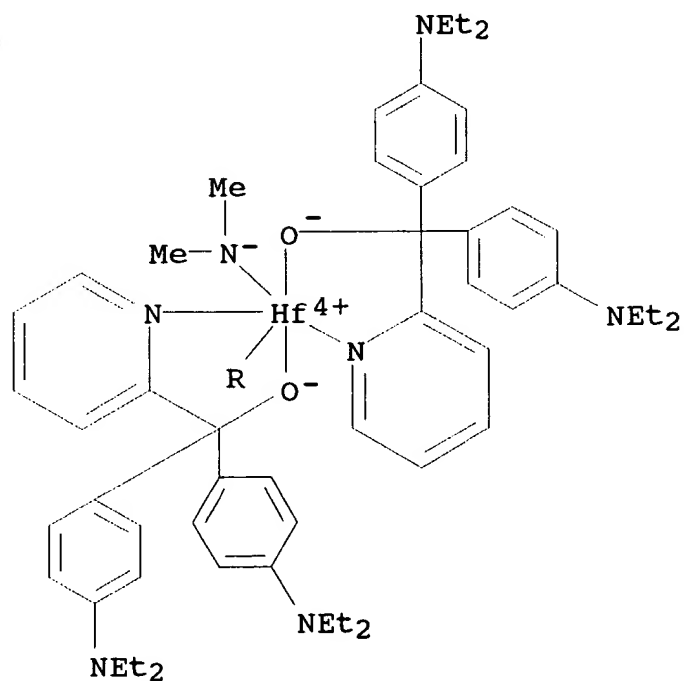


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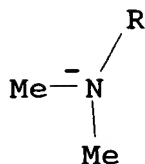


RN 191334-33-5 HCA  
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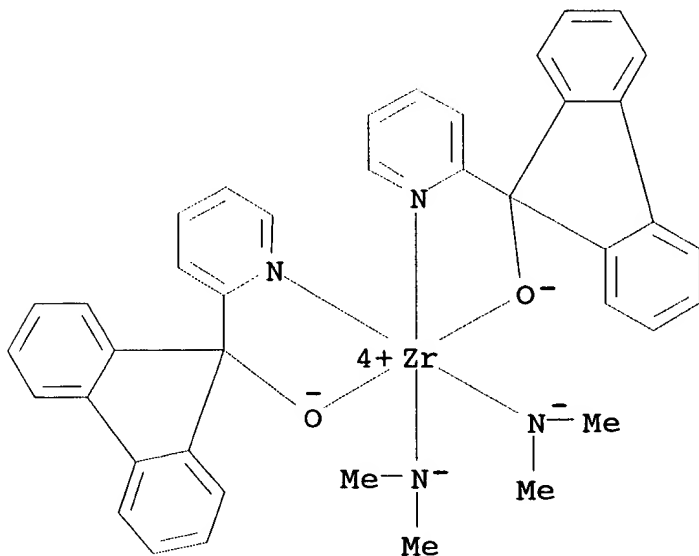


IT 191334-23-3P 191334-27-7P 191334-35-7P  
191334-37-9P

(prepn. of)

RN 191334-23-3 HCA

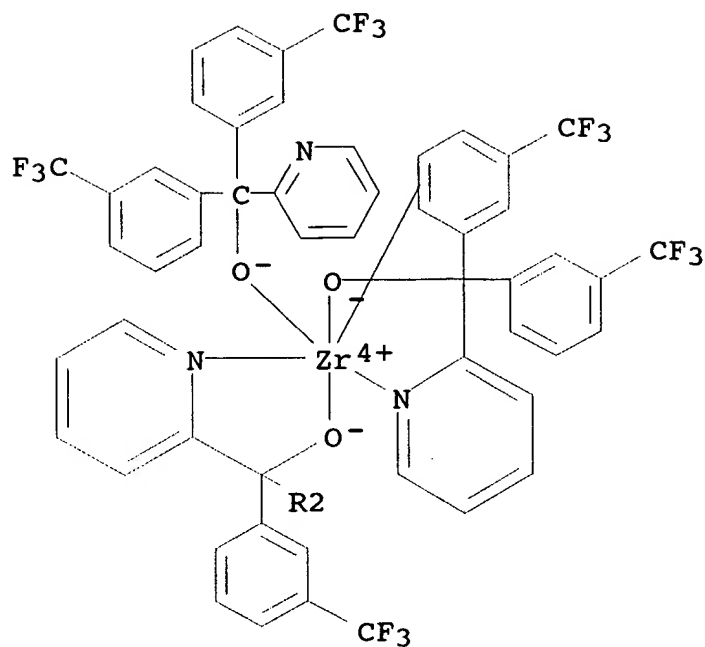
CN Zirconium, bis(N-methylmethanaminato)bis[9-(2-pyridinyl-.kappa.N)-9H-fluoren-9-olato-.kappa.O]-, (OC-6-13)- (9CI) (CA INDEX NAME)



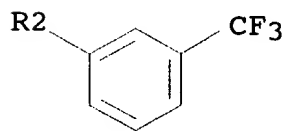
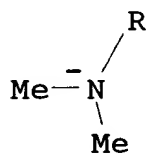
RN 191334-27-7 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2][.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.O2](N-methylmethanaminato)- (9CI) (CA INDEX NAME)

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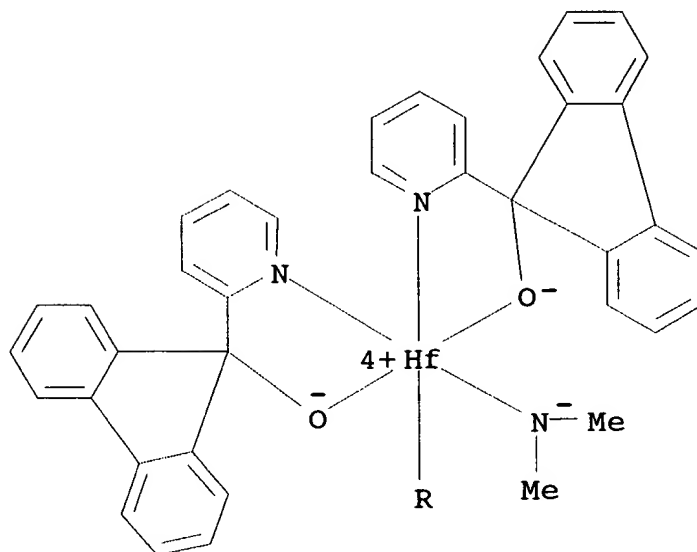
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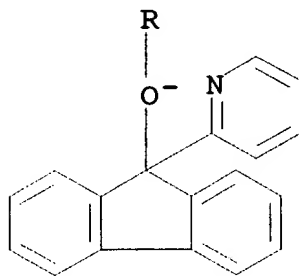
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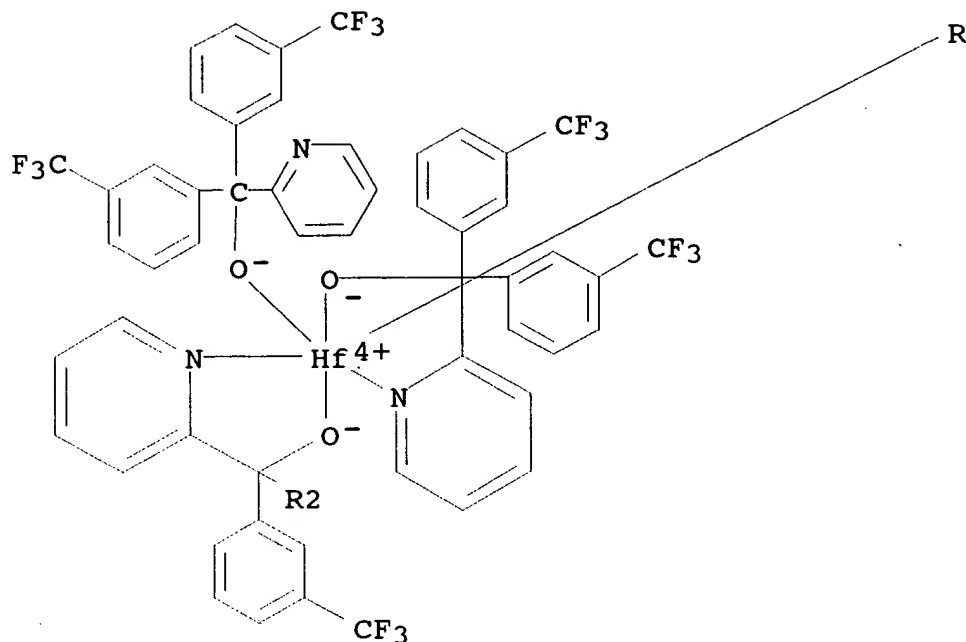


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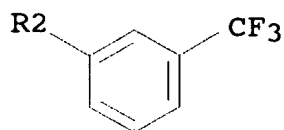
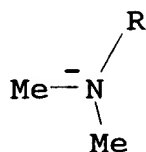


RN 191334-37-9 HCA  
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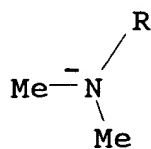
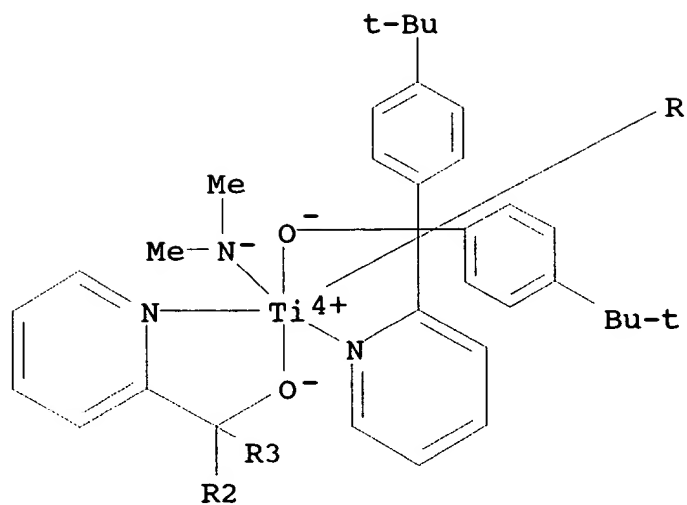
IT 191334-07-3P

(prepn., racemization barrier and **catalyst** for polymn.  
of ethylene)

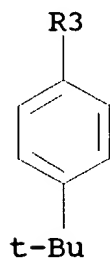
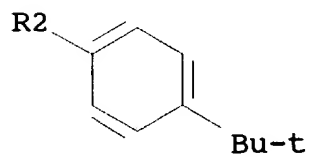
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CN Titanium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-  
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(OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 1-A



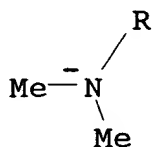
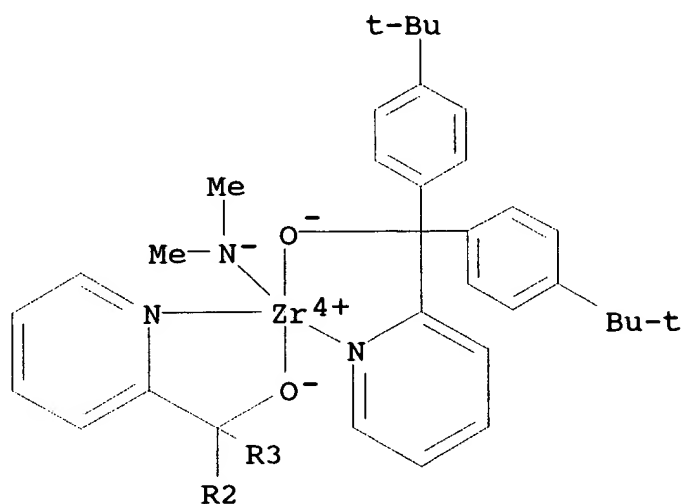
PAGE 2-A



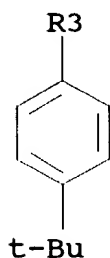
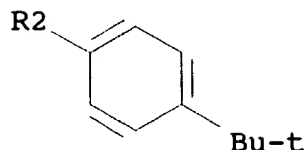
(prepn., racemization barrier, mol. structure and  
**catalyst** for polymn. of ethylene)

RN 191334-21-1 HCA  
 CN Zirconium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-  
 pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,  
 (OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



- CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 23, 27, 35, 67, 75
- ST crystal structure titanium zirconium pyridinemethanolato amido;  
 Group 4 pyridinemethanolato amido prepn structure; titanium  
 pyridinemethanolato amido **catalyst** prepn structure;  
 zirconium pyridinemethanolato amido **catalyst** prepn  
 structure; **olefin polymn catalyst**  
 titanium zirconium pyridinemethanolato; ethylene polymn  
**catalyst** titanium zirconium pyridinemethanolato
- IT Polymerization **catalysts**  
 (**catalytic** polymn. of ethylene by titanium and  
 zirconium and hafnium pyridinemethanolato dimethylamido  
 complexes)
- IT Group IVB element complexes  
 (prepn., crystal structure and racemization in soln. of Group 4  
 pyridinemethanolato dimethylamido complex **olefin**  
**polymn. catalysts**)
- IT 74-85-1, Ethene, reactions 9002-88-4, Polyethylene  
 (**catalytic** polymn. of ethylene by titanium and  
 zirconium and hafnium pyridinemethanolato dimethylamido  
 complexes)
- IT 3275-24-9, Tetrakis(dimethylamido)titanium 19756-04-8,  
 Tetrakis(dimethylamido)zirconium 19782-68-4,  
 Tetrakis(dimethylamido)hafnium  
 (for prepn. of Group 4 pyridinemethanolato dimethylamido complex  
**catalyst** for ethylene polymn.)
- IT 149064-67-5, Bis(4-tert-butylphenyl)-2-pyridylmethanol  
 (for prepn. of Group 4 pyridinemethanolato dimethylamido complex  
**olefin polymn. catalysts**)
- IT 64436-62-0P, 9-(2-Pyridyl)-9-fluorene 95425-83-5P,  
 1-(2-Pyridyl)dibenzosuberone 191333-98-9P, Bis(3-

- (trifluoromethyl)phenyl)-2-pyridylmethanol 191334-00-6P  
 191334-02-8P, Bis(4-(diethylamino)phenyl)-2-pyridylmethanol  
 191334-05-1P, Bis(3,5-bis(trifluoromethyl)phenyl)-2-pyridylmethanol  
 (for prepn. of Group 4 pyridinemethanolato dimethylamido complex  
**olefin polymn. catalysts**)
- IT 90-93-7, 4,4'-Bis(diethylamino)benzophenone 109-04-6,  
 2-Bromopyridine 486-25-9, 9-Fluorenone 1210-35-1,  
 Dibenzosuberone 1868-00-4, 3,3'-Bis(trifluoromethyl)benzophenone  
 3478-90-8, 4,4'-Diphenylbenzophenone 175136-66-0,  
 3,3',5,5'-Tetrakis(trifluoromethyl)benzophenone  
 (for prepn. of pyridinemethanol aryl deriv. and its Group 4  
 pyridinemethanolato dimethylamido complex **catalyst** for  
 ethylene polymn.)
- IT 191334-13-1P 191334-25-5P  
 (prepn. and **catalyst** for polymn. of ethylene)
- IT 191334-39-1P 191334-41-5P  
 (prepn. and crystal structure)
- IT 191334-09-5P  
 (prepn. and crystal structure and **catalyst** for polymn.  
 of ethylene)
- IT 191334-15-3P  
 (prepn. and mol. structure and **catalyst** for polymn. of  
 ethylene)
- IT 191334-11-9P 191334-17-5P 191334-19-7P  
 191334-31-3P 191334-33-5P  
 (prepn. and racemization barrier)
- IT 191334-23-3P 191334-27-7P 191334-29-9P  
 191334-35-7P 191334-37-9P  
 (prepn. of)
- IT 191334-07-3P  
 (prepn., racemization barrier and **catalyst** for polymn.  
 of ethylene)
- IT 191334-21-1P  
 (prepn., racemization barrier, mol. structure and  
**catalyst** for polymn. of ethylene)

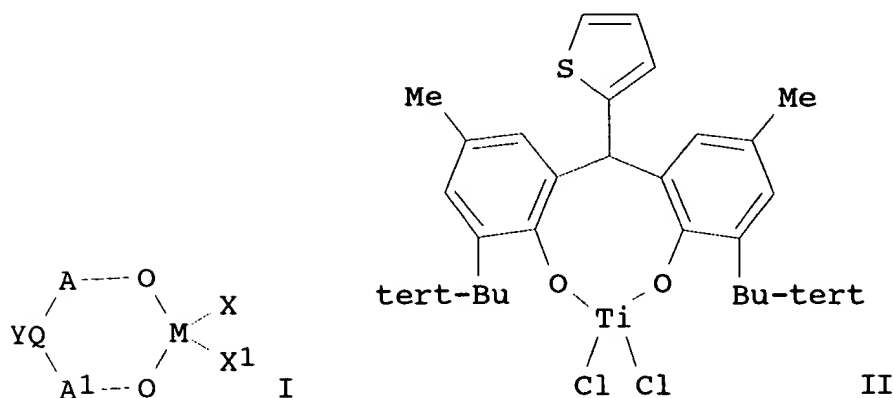
L36 ANSWER 4 OF 7 HCA COPYRIGHT 1998 ACS

126:277883 **Olefin polymerization catalyst**

component, **catalyst** containing it, and use of the  
**catalyst** to produce **olefin polymers**.

Katayama, Hiroaki; Nabika, Masaaki; Imai, Akio; Kawamura, Norio;  
 Hanaoka, Hidenori (Sumitomo Chemical Company, Limited, Japan). Eur.  
 Pat. Appl. EP 761694 A1 970312, 23 pp. DESIGNATED STATES: R: BE,  
 DE, FR, GB, IT, NL. (English). CODEN: EPXXDW. APPLICATION: EP  
 96-305908 960812. PRIORITY: JP 95-205953 950811.

GI



AB The component is represented by the general formula I, in which A and A1 are C1-50 (halogenated) hydrocarbylene optionally bearing an O-contg. substituent, M is a Group 4 transition metal or a lanthanide, Q is a trivalent residue contg. a Group 13-15 element, X and X1 are halogen or C1-20 hydrocarbyl, and Y is a C1-20 (halogenated) hydrocarbon group contg. .gtoreq.1 hetero atom.

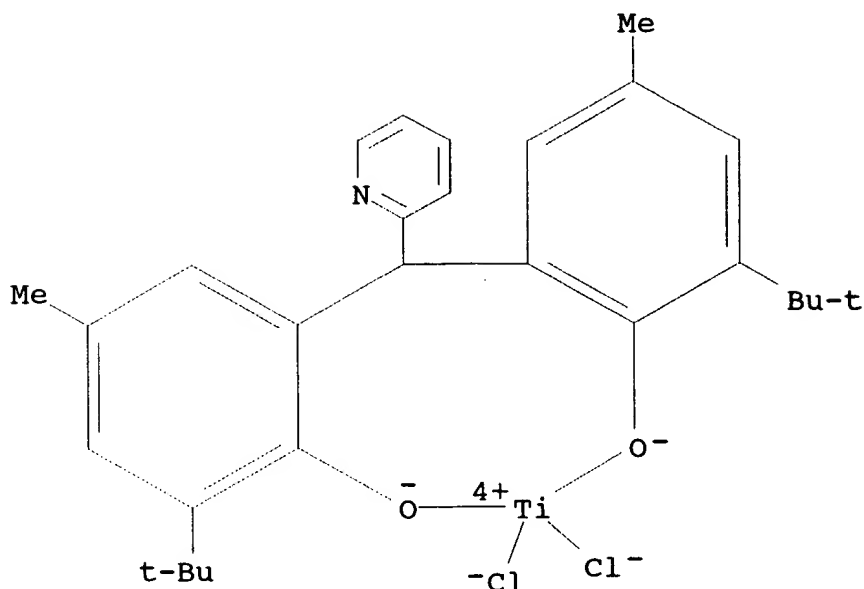
**Catalyst** systems contg. I are highly active at advantageous **polymn.** temps., give **polyolefins** of high mol. wt., and require a reduced amt. of organoaluminum cocatalyst. Thus, 2-tert-butyl-4-methylphenol was treated with MeMgBr, condensed with 2-thiophenecarboxaldehyde, and hydrolyzed to give the bisphenol, which reacted with TiCl<sub>4</sub> to give orange solid II. Copolymn. of ethylene with 1-hexene in toluene at 80.degree. in the presence of Et<sub>3</sub>Al 250, II 5.0, and Ph<sub>3</sub>C<sup>+</sup> -B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub> 15 .mu.mol gave a copolymer with wt.-av. mol. wt. 1.7 .times. 10<sup>5</sup>, mol.-wt. distribution 2.6, and 19.8 short-chain branches per 1000 chain C atoms at a **catalyst** yield of 1.7 .times. 10<sup>6</sup> g copolymer per mol Ti.

IT 188841-53-4P

(prepn. of olefin polymn. catalyst component)

RN 188841-53-4 HCA

CN Titanium, dichloro[[2,2'-(2-pyridinylmethylene)bis[6-(1,1-dimethylethyl)-4-methylphenolato-.kappa.O]](2-)]-, (T-4)- (9CI) (CA INDEX NAME)



IC ICM C08F004-642  
 ICS C08F010-02; C07F007-00  
 CC 35-3 (Chemistry of Synthetic High Polymers)  
 ST **olefin polymn catalyst component;**  
 bisphenol dichlorotitanate **catalyst**  
 IT Linear low-density polyethylenes  
 (**olefin polymn. catalyst component**  
 for manuf. of)  
 IT Aluminoxanes  
 (**olefin polymn. catalyst component**  
 for use with)  
 IT **Polymerization catalysts**  
 (prepn. of **olefin polymn. catalyst**  
 component)  
 IT 25213-02-9P, Ethylene-1-hexene **copolymer**  
 (**olefin polymn. catalyst component**  
 for manuf. of)  
 IT 97-93-8, Triethylaluminum, uses 100-99-2, Triisobutylaluminum,  
 uses 136040-19-2, Triphenylmethyl tetrakis(pentafluorophenyl)borat  
 e  
 (**olefin polymn. catalyst component**  
 for use with)  
 IT 188841-52-3P **188841-53-4P** 188841-54-5P 188841-56-7P  
 188841-57-8P 188841-58-9P 188841-59-0P 188841-61-4P  
 188841-62-5P 188841-63-6P 188841-65-8P  
 (prepn. of **ol fin polymn. catalyst**  
 component)  
 IT 184864-52-6P 184864-66-2P 184864-69-5P 184864-72-0P  
 184864-75-3P 184864-78-6P 184864-84-4P 185151-28-4P



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041 00 01 100012 00 01 100012
(prepn. of ol fin polymn. catalyst
component)

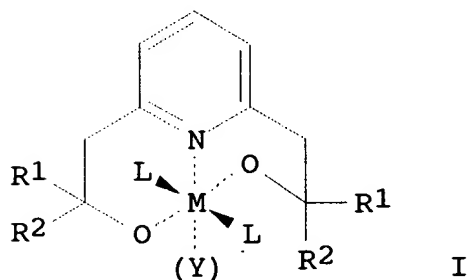
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IT 98-03-3, 2-Thiophenecarboxaldehyde 105-67-9, 2,4-Xylenol  
106-44-5, p-Cresol, reactions 121-00-6, 2-tert-Butyl-4-  
methoxyphenol 497-39-2 1121-60-4, Picolinaldehyde 2409-55-4,  
2-tert-Butyl-4-methylphenol 3541-37-5, 2-  
Benzothiophenecarboxaldehyde 10323-39-4, 4-Bromo-2-tert-  
butylphenol 13679-70-4, 5-Methyl-2-thiophenecarboxaldehyde  
19909-85-4, Dichloro(4-methoxyphenyl)phosphine 26421-44-3,  
2,5-Dimethyl-3-thiophenecarboxaldehyde  
(prepn. of olefin polymn. catalyst  
component)

126:225669 Pyridine-containing transition metal complexes as

olefin polymerization catalysts. Igai,  
Shigeru; Imaoka, Koji; Mitani, Nobuhiro (Ube Industries, Japan).  
Jpn. Kokai Tokkyo Koho JP 09012582 A2 970114 Heisei, 8 pp.  
(Japanese). CODEN: JKXXAF. APPLICATION: JP 95-165160 950630.

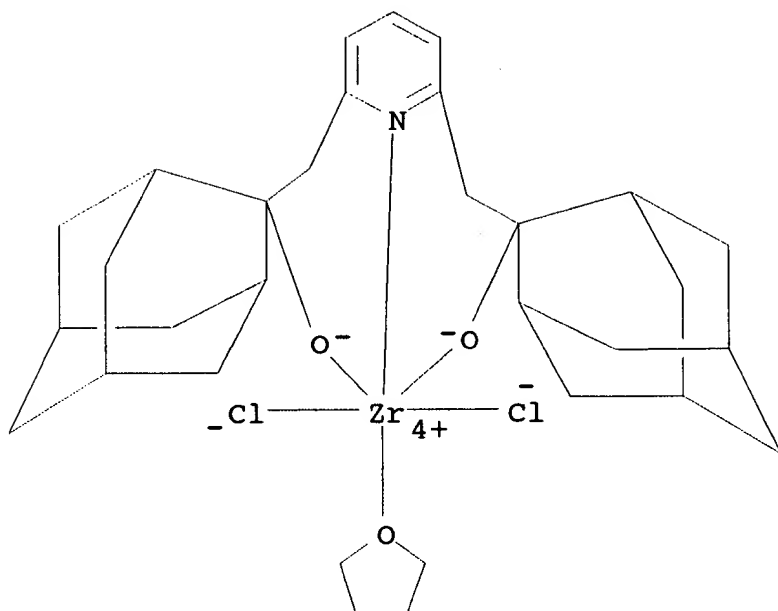
GI



AB The **catalysts** comprise I (R1, R2 = H, hydrocarbyl; R1R2 may form a bridged ring; L = H, halo, hydrocarbyl; M = Group IV metal; Y = heteroatom-contg. electron donor; m = 0, 1, 2; n = 1, 2), and organoaluminum oxy compds. and/or B-contg. ionic compds. Thus, ethylene was polymd. in the presence of I (R1R2 = 2-adamantyl, L = Cl, M = Zr, Y = THF) 5,  $\text{Ph}_3\text{C}^+.\text{cntdot.}(\text{BPh}_4)^- 5$ , and triisobutylaluminum 300 .mu.M in PhMe at 40.degree. to give polymers with Mw 1,320,000, and Mw/Mn 2.7. The **catalyst** activity was 89.4 g/mmol-Zr/h.

(pyridine-contg. transition metal complexes as olefin  
lymn. catalysts)

CN Zirconium, dichloro[[2,2'-[(2,6-pyridinediyl-  
 .kappa.N)bis(methylene)]bis[tricyclo[3.3.1.1<sup>3,7</sup>]decan-2-olato-  
 .kappa.O]](2-)](tetrahydrofuran)-(9CI) (CA INDEX NAME)



- IC ICM C07F007-00  
ICS C07F007-00; C07F007-28; C08F004-76; C08F010-00  
CC 35-3 (Chemistry of Synthetic High Polymers)  
Section cross-reference(s): 27, 67  
ST pyridine transition metal complex **catalyst**; olefin  
pyridine zirconium complex **polymn catalyst**;  
adamantyl pyridine zirconium complex **polymn catalyst**;  
ethylene pyridine zirconium complex **polymn catalyst**  
IT Polymerization **catalysts**  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT Methyl aluminoxanes  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT **Polyolefins**  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT 100-99-2, Triisobutylaluminum, uses 117802-41-2, Trityl  
tetraphenylborate  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT **188032-56-6P**  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT 9002-88-4P, Polyethylene  
(pyridine-contg. transition metal complexes as olefin  
**polymn. catalysts**)  
IT 21959-01-3 149903-53-7

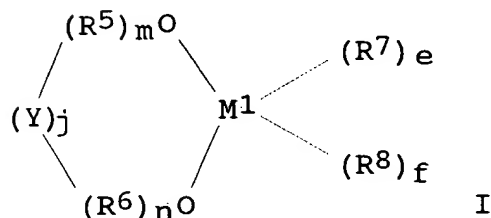
(pyridine-contg. transition metal complexes as **olefin polymn. catalysts**)

L36 ANSWER 6 OF 7 HCA COPYRIGHT 1998 ACS

122:106775 **Catalysts for polymerization of olefins and manufacture of olefin copolymers.**

Yokota, Kiyohiko; Tani, Noriyuki; Watanabe, Masami; Kawasaki, Nobuo (Idemitsu Kosan Co, Japan). Jpn. Kokai Tokkyo Koho JP 06192330 A2 940712 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 93-257671 930921. PRIORITY: JP 92-279372 920924.

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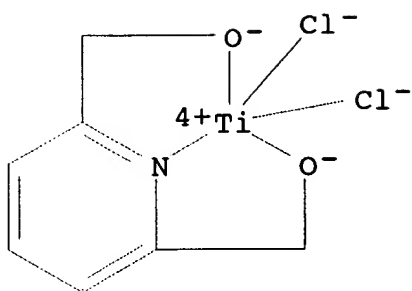
AB **Olefin copolymers** are manufd. with **catalysts** comprising transition metal compds. I [M1 = Group 3-10 or lanthanide metal; R5, R6 = C1-20 hydrocarbylene; R7, R8 = .sigma.-bonding ligand, chelating ligand, Lewis base; Y = C1-20 hydrocarbylene, XR9R10, O, S; R9, R10 = C1-20 hydrocarbyl; X = C, N, S, P, Si; e, f = 0-2; e + f = (valence of M1) - 2; j = 0-4; m, n = 0, 1], ionic compds. forming complexes with I, and optional organoaluminum compds. Thus, 40 mL 1-octene was copolymd. with ethylene at 80.degree. and 8 atm in PhMe in a 1-L autoclave in the presence of iso-Bu3Al, [2,2'-thiobis(6-tert-butyl-4-methylphenoxy)]titanium dichloride, and PhNMe2HB(C6F5)4 for 1 h to give 0.60 g copolymer showing intrinsic viscosity 9.25 dL/g and m.p. 79.degree..

IT 160758-51-0 160758-52-1

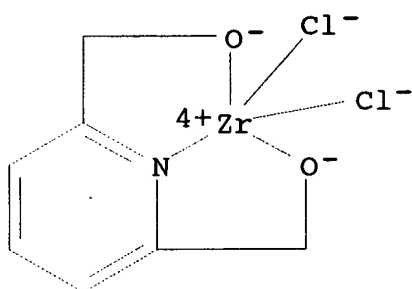
(transition metal-ionic compd. **catalysts** for **polymn. of olefins**)

RN 160758-51-0 HCA

CN Titanium, dichloro[2,6-pyridinedimethanolato(2-)-N1,O.alpha.,O.alpha.]- (9CI) (CA INDEX NAME)



RN 160758-52-1 HCA  
 CN Zirconium, dichloro[2,6-pyridinedimethanolato(2-)-  
 N1,O.alpha.,O.alpha.]- (9CI) (CA INDEX NAME)



IC ICM C08F010-00  
 ICS C08F004-642  
 CC 35-3 (Chemistry of Synthetic High Polymers)  
 ST **olefin polymn catalyst** transition  
 metal; complex transition metal **catalyst** polymn  
 IT Polymerization **catalysts**  
 (transition metal-ionic compd. **catalysts** for  
**polymn. of olefins**)  
 IT Alkenes, preparation  
 (polymers, transition metal-ionic compd. **catalysts** for  
**polymn. of olefins**)  
 IT 100-99-2, Triisobutylaluminum, uses 1109-15-5,  
 Tris(pentafluorophenyl)boron 13523-46-1 104901-00-0  
 104901-01-1 110301-92-3 111215-59-9, 2,2'-Thiobis(6-tert-butyl-4-  
 methylphenoxy)titanium dichloride 118612-00-3 159804-08-7,  
 Dibenzyl[2,2'-thiobis(6-tert-butyl-4-methylphenoxy)]titanium  
 160481-72-1 **160758-51-0 160758-52-1**  
 160758-53-2 160758-54-3  
 (transition metal-ionic compd. **catalysts** for  
**polymn. of ol fins**)  
 IT 9002-88-4P 26221-73-8P  
 (transition metal-ionic compd. **catalysts** for  
**polymn. of ol fins**)

L36 ANSWER 7 OF 7 HCA COPYRIGHT 1998 ACS

121:280477 Polymer-immobilized manganese(III)-Schiff base complexes for **catalytic** epoxidation of olefins. Fujii, Yuki; Ebina, Fujio; Yanagisawa, Manabu; Matsuoka, Hitoshi; Kato, Tohru (Fac. Sci., Ibaraki Univ., Ibaraki, 310, Japan). J. Inorg. Organomet. Polym., 4(3), 273-88 (English) 1994. CODEN: JIOPE4. ISSN: 1053-0495. OTHER SOURCES: CASREACT 121:280477.

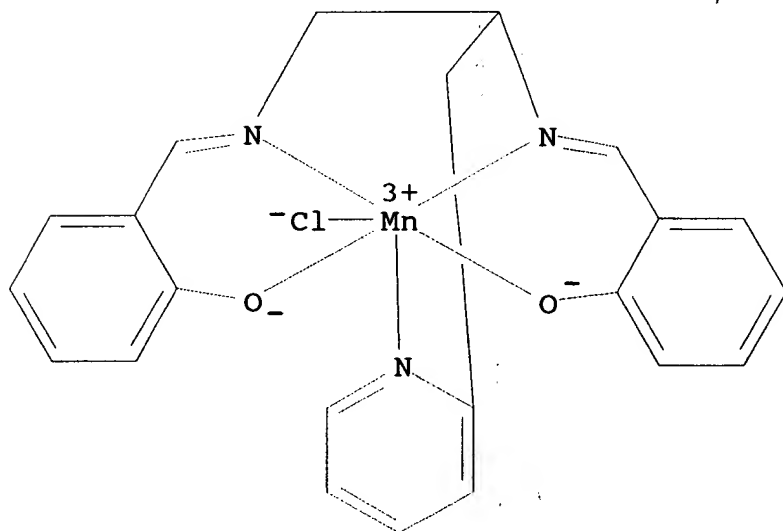
AB Polymer-linked manganese(III)-salen-type Schiff base complexes were prepd. by the copolymer. of functionalized Schiff base, styrene, and divinylbenzene at various mixing ratios (1:10:0-1:12:4), followed by introduction of Mn(III) ion. The materials **catalyzed** epoxidn. of cyclohexene with iodosylbenzene in CH<sub>2</sub>Cl<sub>2</sub> as rapidly as the monomer complexes. The max. total turnover reached 170, which is about 13 times higher than that of the monomer. The lifetime of polymer **catalysts** is discussed in terms of crosslinking and solvent effects.

IT 158989-20-9

(prepn. of polymer-immobilized manganese-Schiff base complexes for **catalytic** epoxidn. of olefins)

RN 158989-20-9 HCA

CN Manganese, chloro[[2,2'-[[1-(2-pyridinylmethyl)-1,2-ethanediyl]bis(nitrilomethylidene)]bis[phenolato]](2-)-N,N',N'',O,O']-, (OC-6-65)-(9CI) (CA INDEX NAME)



CC 27-2 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 67, 78

ST polymer immobilized manganese Schiff base complex; epoxidn  
**catalyst olefin polymer immobilized**  
manganese

IT Alkenes, reactions

(**catalytic** epoxidn. of)  
 IT Epoxidation **catalysts**  
 Polymer-supported reagents  
 Solvent effect  
 (prepn. of polymer-immobilized manganese-Schiff base complexes  
 for **catalytic** epoxidn. of olefins)  
 IT 27658-88-4 53177-12-1 73808-82-9 80778-81-0 158989-19-6  
**158989-20-9** 158989-21-0 158989-22-1  
 (prepn. of polymer-immobilized manganese-Schiff base complexes  
 for **catalytic** epoxidn. of olefins)  
 IT 7439-96-5DP, Manganese, polymer supported salen and styrene  
 divinylbenzene complexes 27658-88-4DP, styrene divinylbenzene  
 polymer supported 53177-12-1DP, styrene divinylbenzene polymer  
 supported 158959-83-2DP, manganese chloride complexes  
 158959-84-3DP, manganese chloride complexes 158959-85-4DP,  
 manganese chloride complexes 158959-86-5DP, manganese chloride  
 complexes  
 (prepn. of polymer-immobilized manganese-Schiff base complexes  
 for **catalytic** epoxidn. of olefins)  
 IT 90-02-8, Salicylaldehyde, reactions 107-15-3, 1,2-Ethanediamine,  
 reactions 110-83-8, Cyclohexene, reactions 536-80-1,  
 Iodosylbenzene 58813-73-3 158959-80-9 158959-82-1  
 (prepn. of polymer-immobilized manganese-Schiff base complexes  
 for **catalytic** epoxidn. of olefins)  
 IT 158959-81-0P 158959-83-2P 158959-84-3P 158959-85-4P  
 158959-86-5P  
 (prepn. of polymer-immobilized manganese-Schiff base complexes  
 for **catalytic** epoxidn. of olefins)

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(FILE 'REGISTRY' ENTERED AT 14:16:32 ON 04 AUG 1998)

FILE 'HCA' ENTERED AT 14:17:22 ON 04 AUG 1998

L38 48 S L37 NOT 1995-1997/PY

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L38 ANSWER 1 OF 48 HCA COPYRIGHT 1998 ACS

123:73254 New mixed complexes of Zr (IV) with mono and multidentate  
 ligands. Tarafder, M. T. H.; Islam, M. Shamsul; Bhattacharjee, P.;  
 Quraishi, S. B. (Department of Chemistry, Rajshahi University,  
 Rajshahi, Bangladesh). Pak. J. Sci. Ind. Res., 37(4), 126-8  
 (English) 1994. CODEN: PSIRAA. ISSN: 0030-9885.

AB Several new complexes of Zr (IV) contg. a no. of monodentate and  
 multidentate org. ligands were synthesized and characterized. The  
 complexes have the compns., [Zr(O)Cl<sub>2</sub>(en).H<sub>2</sub>O], [Zr(O)Cl<sub>2</sub>.2L.H<sub>2</sub>O],  
 [Zr.L'<sub>3</sub>Cl] and [Zr(O)Cl<sub>2</sub>.L'] [en = ethylenediamine; L = OPPh<sub>3</sub>,  
 OAsPh<sub>3</sub>, pyridine or aniline; HL' = 8-hydroxyquinoline,  
 o-aminophenol, L' = diethylenetriamine and triethylenetetramine].  
 The molar conductance data indicate that complexes [Zr(C<sub>9</sub>H<sub>6</sub>NO)<sub>3</sub>Cl]

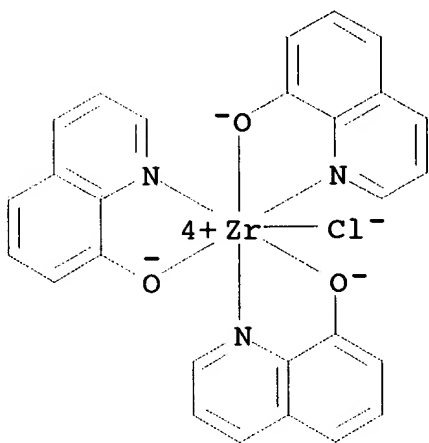
and  $[\text{Zr}(\text{C}_6\text{H}_4\text{NH}_2\text{O})_3\text{Cl}]$  are 1:1 electrolytes but all other complexes behave as 2:1 electrolytes. The exptl. data are consistent with 6-fold coordination of Zr (IV) ion in all the complexes excepting  $[\text{Zr}(\text{C}_9\text{H}_6\text{NO})_3\text{Cl}]$   $[\text{Zr}(\text{C}_6\text{H}_4\text{NH}_2\text{O})_3\text{Cl}]$  and  $[\text{Zr}(\text{O})\text{Cl}_2\text{.tet}]$  which are seven coordinated.

IT **165182-50-3P**

(prepn. of)

RN 165182-50-3 HCA

CN Zirconium, chlorotris(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

IT 165182-45-6P 165182-46-7P 165182-47-8P 165182-48-9P

165182-49-0P **165182-50-3P** 165182-51-4P 165182-52-5P

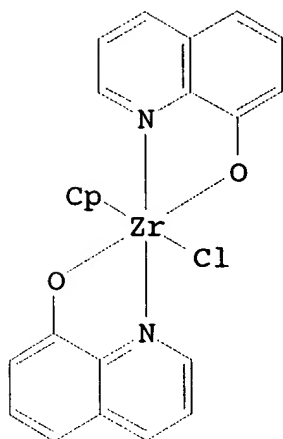
165182-53-6P

(prepn. of)

L38 ANSWER 2 OF 48 HCA COPYRIGHT 1998 ACS

120:270657 Dissociation of zirconocene hydridochloride. Zhang, YunWen; Bai, LingJun; Xu, YuMing; Li, JiangSheng; Wang, JiTao (Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China). Prog. Nat. Sci., 3(1), 83-8 (English) 1993. CODEN: PNASEA. OTHER SOURCES: CASREACT 120:270657.

GI



I

AB Dissozn. of zirconocene hydrido-chloride,  $\text{CpZrHCl}$ , was examd. by substitution reaction with phosphorus and nitrogen ligands, L, under thermal or photolytic conditions to give Zr(III) as  $\text{Cp}_2\text{ZrClL}$  complex stable for several weeks without oxygen.  $\text{Cp}_2\text{ZrClL}$  decomp. in air to give  $(\text{Cp}_2\text{ZrCl})_2\text{O}$  and L. It was concluded that Zr-H bond experiences homolytic reaction under heating and irradiation without active hydrogen. The heterolytic reaction of  $\text{Cp}_2\text{ZrClH}$  with nitrogen-contg. hydroxyl compds. was shown to give Zr-contg. heterocyclic organometallics, e.g., I. I was characterized by x-ray crystallog.

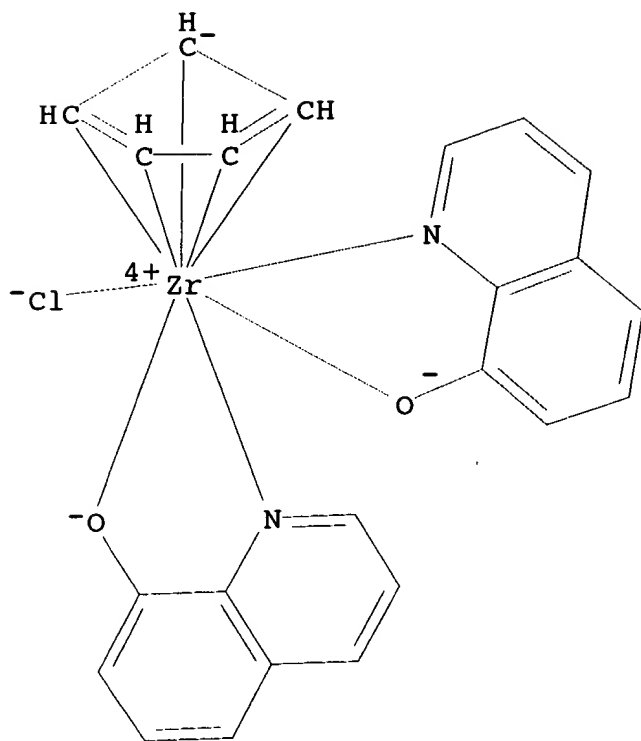
IT 12114-15-7P

(prepn. and crystal and mol. structure of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



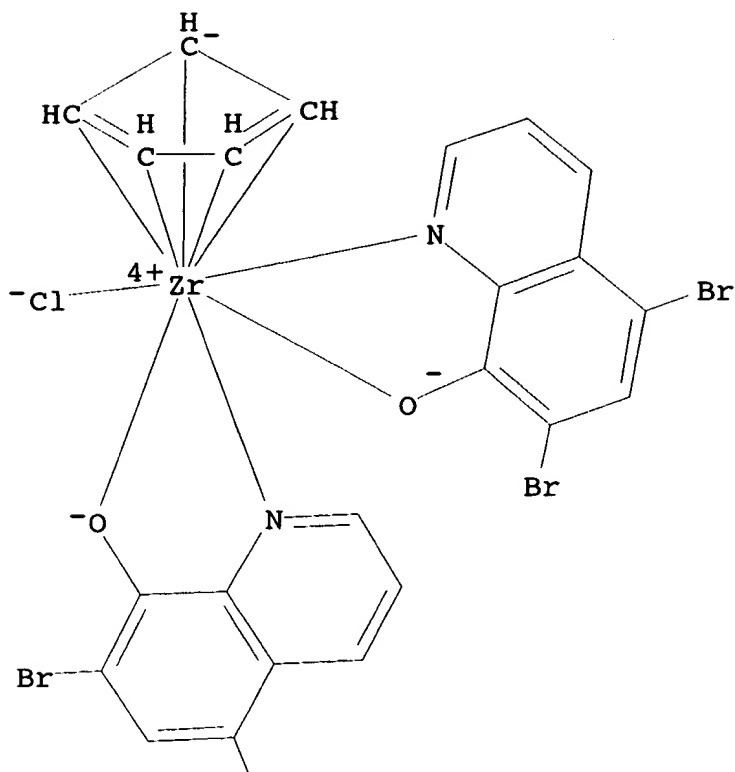


IT 148484-15-5P 148484-16-6P 154426-19-4P  
(prepn. of)

RN 148484-15-5 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)

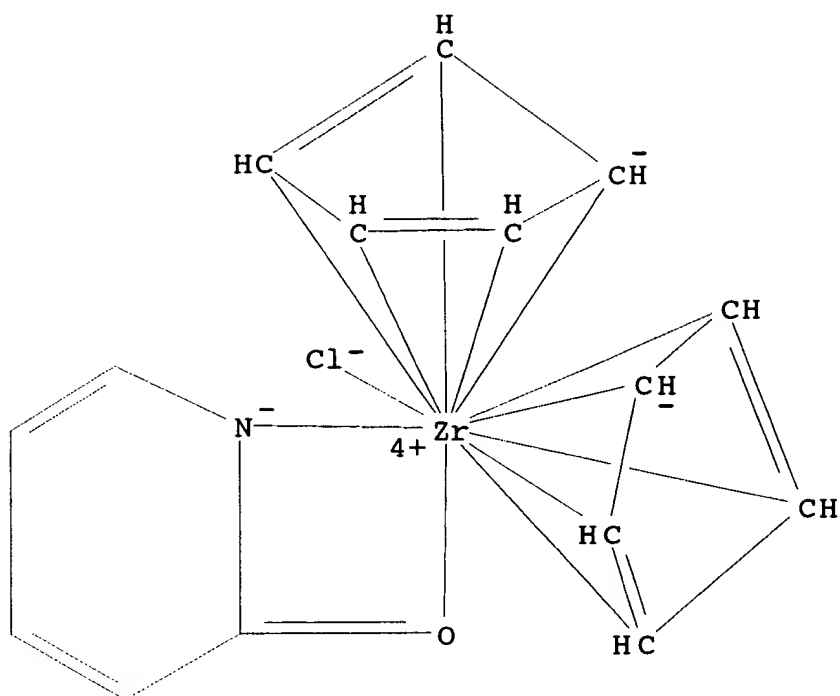
PAGE 1-A



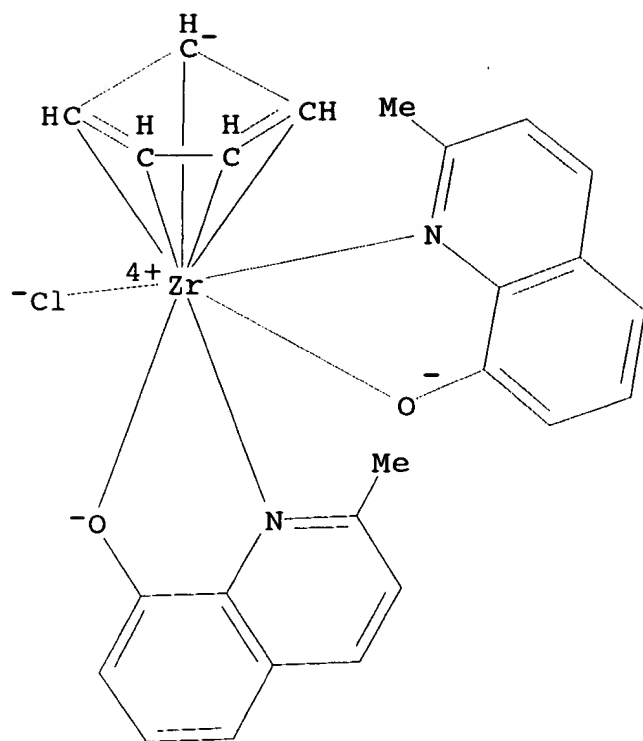
PAGE 2-A

Br

RN 148484-16-6 HCA  
 CN Zirconium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-pyridinonato-N1,O2)- (9CI) (CA INDEX NAME)



RN 154426-19-4 HCA  
 CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(2-methyl-8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 75

IT **12114-15-7P**

(prepn. and crystal and mol. structure of)

IT 12097-04-0P **148484-15-5P 148484-16-6P**  
**148484-17-7P 154426-19-4P**

(prepn. of)

L38 ANSWER 3 OF 48 HCA COPYRIGHT 1998 ACS

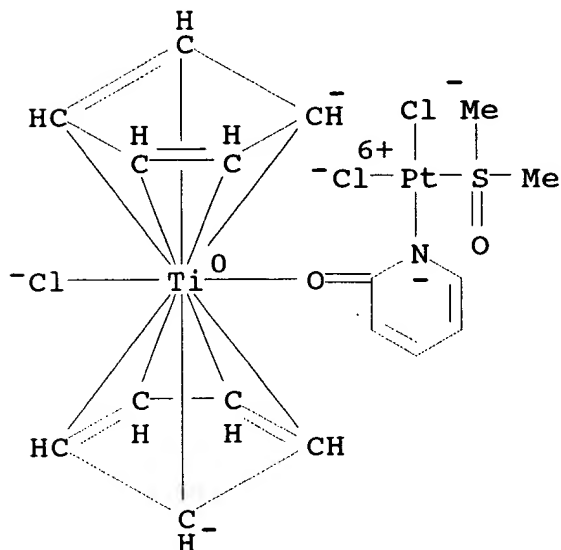
119:84507 Heterobimetallic platinum-titanium complexes: potential anticancer drugs. Berardini, M.; Emge, T. J.; Brennan, J. G. (Dep. Chem., Rutgers Univ., Piscataway, NJ, 08855-0939, USA). Inorg. Chem., 32(12), 2724-8 (English) 1993. CODEN: INOCAJ. ISSN: 0020-1669. OTHER SOURCES: CJACS-IMAGE; CJACS.

AB Heterobimetallic complexes contg. titanocene chloride and trans-PtCl<sub>2</sub>(DMSO) functional groups were prepd. by bridging the metal centers with hydroxypyridine (HL), to explore the possibility that a chelate effect will enhance DNA-metal binding affinity and chemotherapeutic effectiveness. The structure of trans-PtCl<sub>2</sub>(DMSO)(L-2-Ti(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Cl) was detd.: monoclinic, space group Cc, a 6.958(2), b 18.047(3), c 33.217(5) .ANG., .beta. 92.04(2).degree., Z = 4, R = 0.049, R<sub>w</sub> = 0.067. Both metal coordination environments are virtually identical to related monometallic complexes.

IT **149063-33-2P**

(prepn. and crystal structure and potential anticancer activity of)

RN 149063-33-2 HCA  
 CN Titanium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)[dichloro[sulfinylbis[methane]-S]platinum][.mu.-(2(1H)-pyridinonato-N1:O2)]-, stereoisomer (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 1, 29, 75

IT 149063-33-2P

(prepn. and crystal structure and potential anticancer activity of)

L38 ANSWER 4 OF 48 HCA COPYRIGHT 1998 ACS

119:49507 Syntheses and characterization of heterocyclic compounds of zirconium(IV). Wang, Jitao; Zhang, Yunwen; Xiu, Yuming; Li, Jiangsheng; Gong, Yousheng (Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China). Chem. Res. Chin. Univ., 8(3), 212-18 (English) 1992. CODEN: CRCUED. OTHER SOURCES: CASREACT 119:49507.

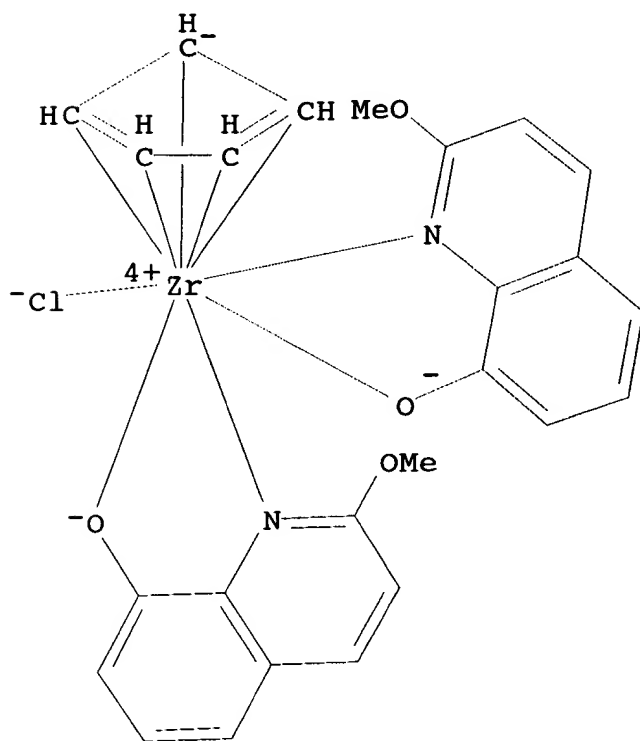
AB The Zr-H bond of zirconocene hydridechloride was heterolyzed at room temp. by 5 compds. contg. nitrogen and an hydroxyl group to give Cp(η)2ZrCl (I, QH = 8-quinolinol, 2-methoxy-8-quinolinol, 5,7-dibromo-8-quinolinol, 2-pyridol, ethanolamine) which were characterized by elemental anal., IR, and 1H NMR spectroscopy. The mol. structure of I (QH = 8-quinolinol) was confirmed by x-ray diffraction detn. The coordination polyhedron around the Zr atom can be described as a distorted octahedron. The Zr-N bonds of 0.2364(3) and 0.2377(4) nm suggest that they are coordination bonds. The two planar 8-quinolinoyl groups act as bidentate ligands chelated with Zr, forming a dihedral angle of 108.4(1).degree..

IT 148484-14-4P 148484-15-5P 148484-16-6P

(prepn. and fluorescence of)

RN 148484-14-4 HCA

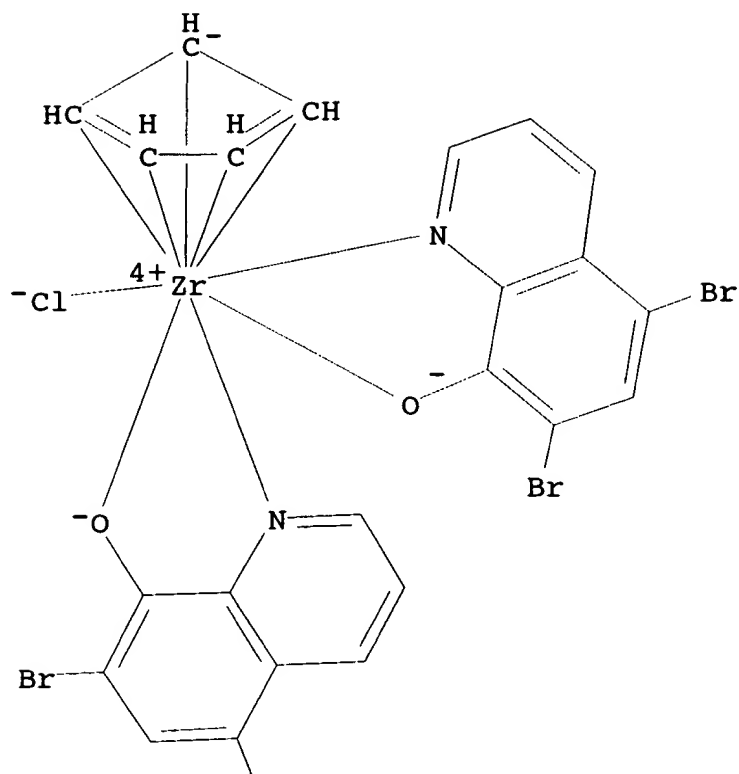
CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(2-methoxy-8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



RN 148484-15-5 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)

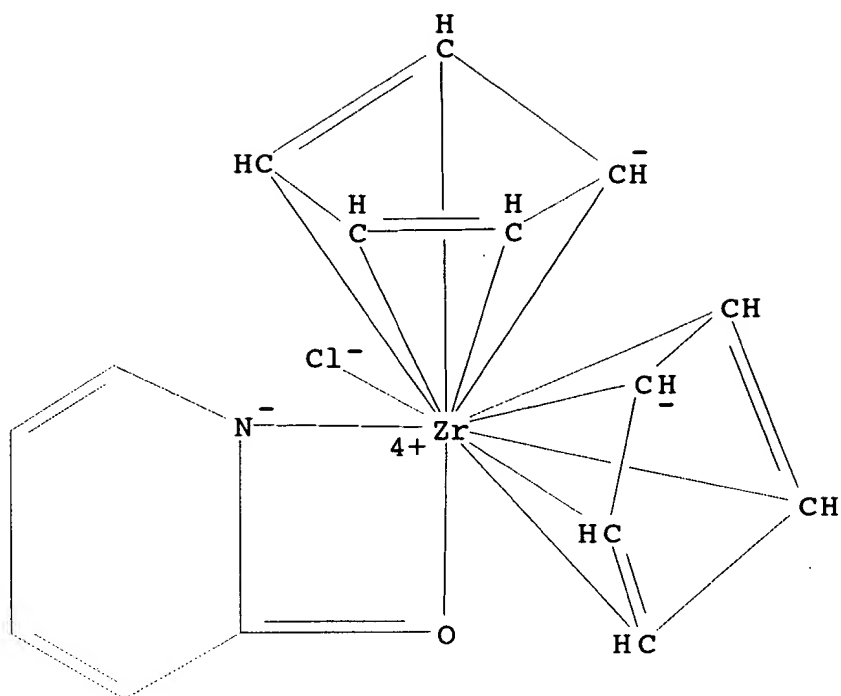
PAGE 1-A



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RN 148484-16-6 HCA  
 CN Zirconium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-pyridinonato-N1,O2)-(9CI) (CA INDEX NAME)



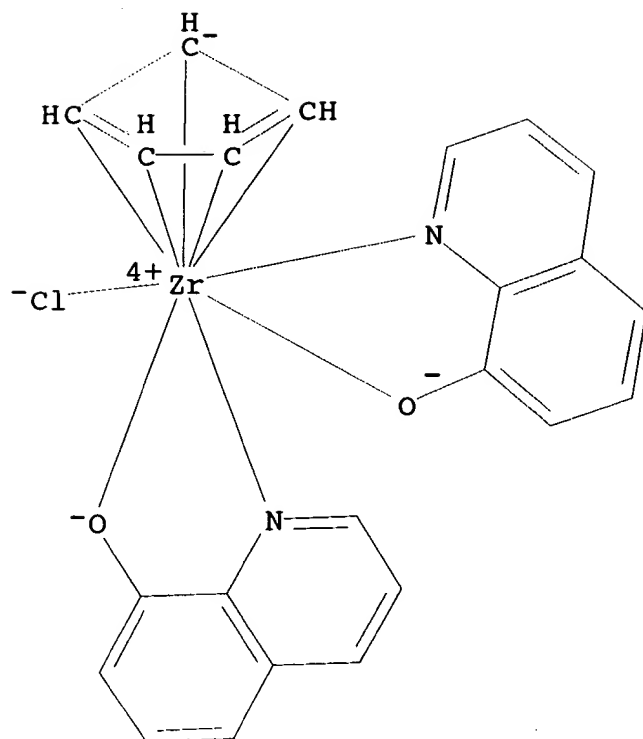
IT 12114-15-7P

(prepn., crystal structure, and fluorescence of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)





CC 29-10 (Organometallic and Organometalloidal Compounds)  
Section cross-reference(s): 75

IT 148484-14-4P 148484-15-5P 148484-16-6P  
148484-17-7P

(prepn. and fluorescence of)

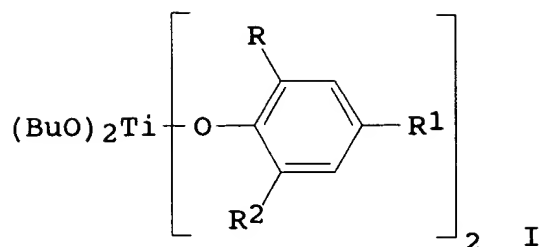
IT 12114-15-7P

(prepn., crystal structure, and fluorescence of)

L38 ANSWER 5 OF 48 HCA COPYRIGHT 1998 ACS

116:21104 Hydrosilylation of titanates containing allyl aromatic radicals. Suvorov, A. L.; Khonina, T. G.; Kodess, M. I.; Podol'skii, A. V. (Inst. Khim., Sverdlovsk, USSR). Zh. Obshch. Khim., 61(6), 1383-9 (Russian) 1991. CODEN: ZOKHA4. ISSN: 0044-460X.

GI



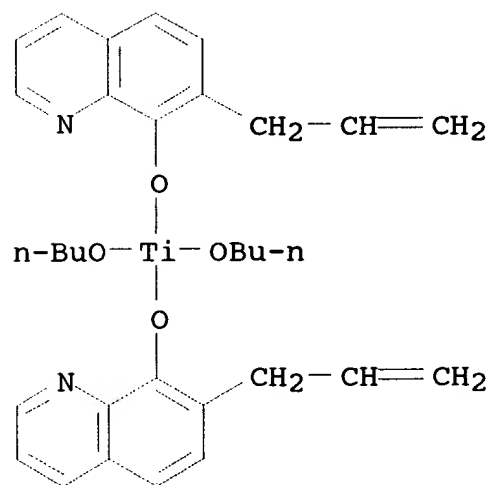
AB The hydrosilylation reactivity of titanates I ( $\text{R} = \text{R}^2 = \text{Me}$ ,  $\text{R}^1 = \text{allyl}$ ;  $\text{R} = \text{R}^1 = \text{H}$ ,  $\text{R}^2 = \text{allyl}$ ) by  $\text{MeSiHR}32$  ( $\text{R}^3 = \text{Ph}$ ,  $\text{CH}_2\text{Ph}$ ,  $\text{C}_5\text{H}_{11}$ ) was governed by steric effects, and the extent of hydrosilylation depended on the extent of allyl-propenyl isomerization.

IT **138142-58-2**

(hydrosilylation of)

RN 138142-58-2 HCA

CN Titanium, dibutoxybis[7-(2-propenyl)-8-quinolinolato-O]-, (T-4)-(9CI) (CA INDEX NAME)



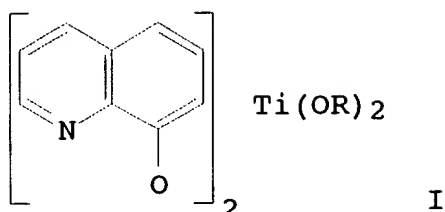
CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 16709-91-4, Dibenzylmethylvinylsilane 18042-43-8 132410-71-0  
 138142-57-1 **138142-58-2** 138142-59-3 138166-09-3  
 (hydrosilylation of)

L38 ANSWER 6 OF 48 HCA COPYRIGHT 1998 ACS

109:129860 Manufacture of titanoxane-siloxanes from silicic acid and titanium alkoxides. Misono, Takahisa; Abe, Yoshisaki; Hikita, Michiro; Nagao, Yukinori (Nissan Chemical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 63056530 A2 880311 Showa, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 86-200877 860827.

GI



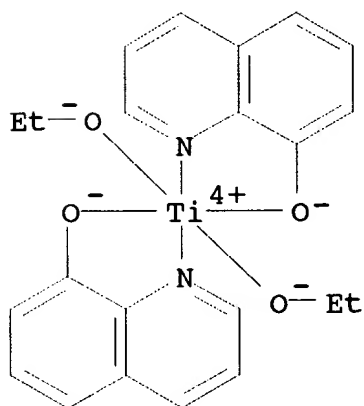
AB Titanoxane-siloxanes, non-gel solids at ambient temps., stable, and convertible by hydrolytic or thermal polycondensation into inorg. polymers, are prepd. by refluxing bis(8-oxyquinolinato)titanium dialkoxides I ( $\text{R} = \text{C1-4 alkyl}$ ) or  $(\text{R}_2\text{COCH:CR}_1\text{O})_2\text{Ti}(\text{OR})_2$  (II;  $\text{R}_1 = \text{C1-3 alkyl, Ph}$ ;  $\text{R}_2 = \text{C1-3 alkyl, C1-3 alkoxy, Ph, OPh, OCH}_2\text{Ph}$ ;  $\text{R}_1$  and  $\text{R}_2$  are not Me simultaneously) with silicic acid at mol ratio  $\text{SiO}_2/\text{TiO}_2$  0.25-4 in a solvent. A THF soln. (11.8 parts) of silicic acid (0.6 part  $\text{SiO}_2$ ) and 30 parts  $\text{Me}_2\text{CO}$  soln. of 3.9 parts II ( $\text{R} = \text{Bu}$ ,  $\text{R}_1 = \text{Me}$ ,  $\text{R}_2 = \text{OEt}$ ) were mixed and refluxed for 30 min to give 4.3 parts polymer which showed mol ratio  $\text{SiO}_2/\text{TiO}_2$  1, and which was pulled into a 110-cm-long thread by a glass rod, and did not gel and retained its threading property when left in air for 120 h.

IT 23329-68-2

(polycondensation of, with silicic acid, titanoxane-siloxanes from)

RN 23329-68-2 HCA

CN Titanium, diethoxybis(8-quinolinolato-N1,O2)- (9CI) (CA INDEX NAME)



IC ICM C08G077-58

CC 35-4 (Chemistry of Synthetic High Polymers)

IT 20753-28-0 23329-68-2 116075-48-0, Bis(ethyl-3-phenyl-3-oxopropanoate)titanium diisopropoxide

(polycondensation of, with silicic acid, titanoxane-siloxanes from)

L38 ANSWER 7 OF 48 HCA COPYRIGHT 1998 ACS

105:202079 Composition and stability of niobium(V), zirconium(IV), yttrium(III) and lanthanum(III) chelates with 7-nitroso-8-quinolinone-5-sulfonate. El-Haty, M. T.; Adam, F. A. (Chem. Dep., Fac. Sci., Aswan, Egypt). Bull. Soc. Chim. Fr. (3), 351-4 (English) 1986. CODEN: BSCFAS. ISSN: 0037-8968.

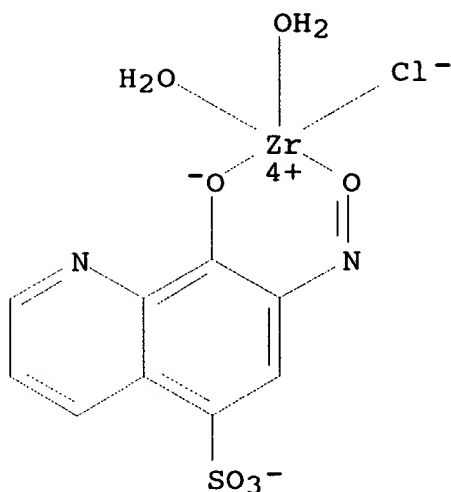
AB New Nb(V), Zr(IV), Y(III) and La(III) chelates obtained from disodium 7-nitroso-8-quinolinone-5-sulfonate were studied by spectrophotometric, conductimetric and potentiometric methods. The solid chelates were prepd. and their IR spectra and elemental anal. were discussed. The ligand is bonded to the metal ion through the O atoms of nitroso and hydroxy groups. The apparent stability consts. of the complexes formed in soln. were also detd. spectrophotometrically and potentiometrically.

IT 105194-69-2P 105212-59-7P

(prepn. and IR spectrum of)

RN 105194-69-2 HCA

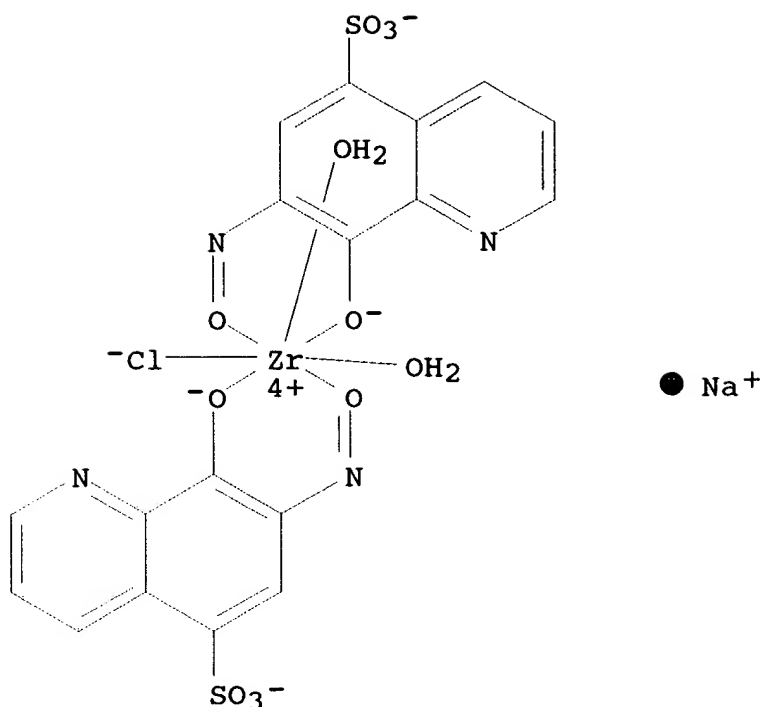
CN Zirconium(1+), diaquachloro[8-hydroxy-7-nitroso-5-quinolinesulfonato(2-)-07,08]-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

RN 105212-59-7 HCA

CN Zirconate(1-), diaquachlorobis[8-hydroxy-7-nitroso-5-quinolinesulfonato(2-)-07,08]-, sodium (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 68

IT 105177-47-7P 105177-48-8P 105177-50-2P 105177-51-3P

105194-68-1P **105194-69-2P** 105194-70-5P

**105212-59-7P**

(prepn. and IR spectrum of)

L38 ANSWER 8 OF 48 HCA COPYRIGHT 1998 ACS

103:160633 Synthesis and characterization of .eta.5-cyclopentadienyl chloro zirconium(IV) complexes of 8-hydroxyquinoline N-oxide.

Sharma, S.; Sharma, A.; Goyal, K. C.; Kaushik, N. K. (Dep. Chem., Univ. Delhi, Delhi, India). Bull. Soc. Chim. Fr. (11-12, Pt. 1), 327-8 (English) 1984. CODEN: BSCFAS. ISSN: 0037-8968.

AB (.eta.5-C5H5)Zr(L)2Cl (LH = 8-hydroxyquinoline N-oxide, 5-nitro-, 5,7-dinitro-, 5,7-dibromo- or 5-phenylazo-8-quinoline N-oxides) were synthesized in non-aq. medium by the reaction (.eta.5-C5H5)2ZrCl2 with 8-hydroxyquinoline N-oxide and its substituted derivs. The N-oxides behave as unineg. bidentate ligands and Zr is hexacoordinate in all the complexes.

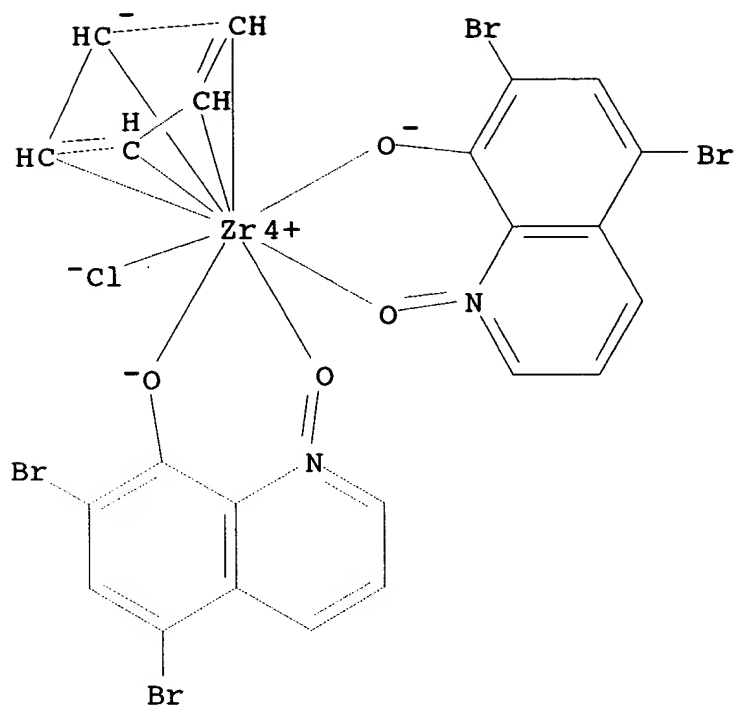
IT **98606-19-0P 98606-20-3P 98606-21-4P**

**98606-22-5P 98606-31-6P**

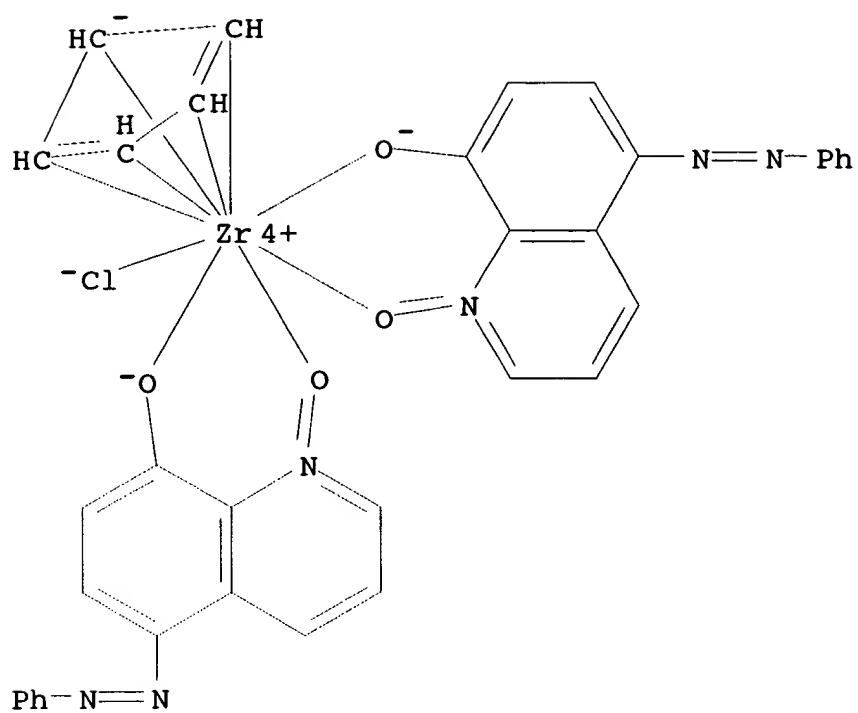
(prepn. and spectra of)

RN 98606-19-0 HCA

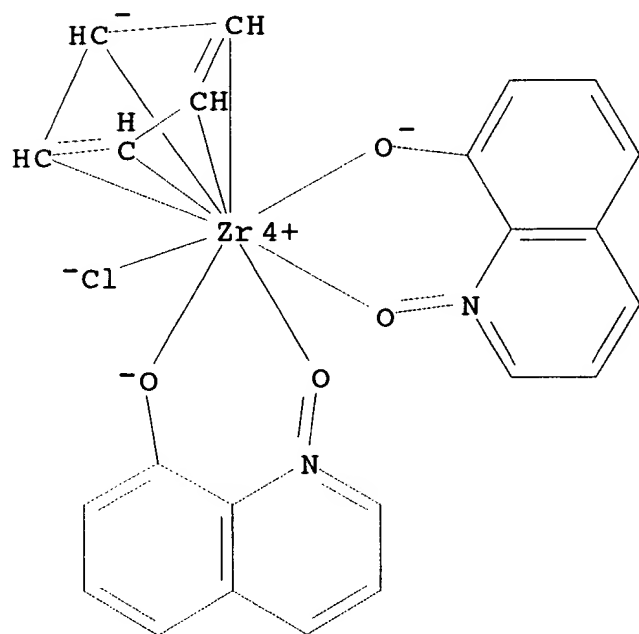
CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinol 1-oxidato-O,O')- (9CI) (CA INDEX NAME)



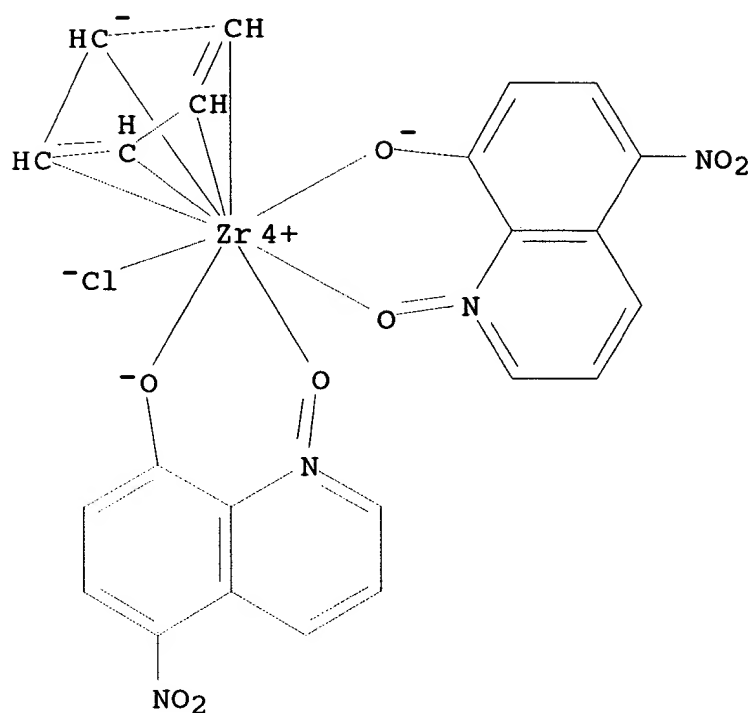
RN 98606-20-3 HCA  
 CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis[5-(phenylazo)-8-quinolinol 1-oxidato-O,O']- (9CI) (CA INDEX NAME)



RN 98606-21-4 HCA  
 CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl) (8-quinolinol  
 1-oxidato-O,O')- (9CI) (CA INDEX NAME)

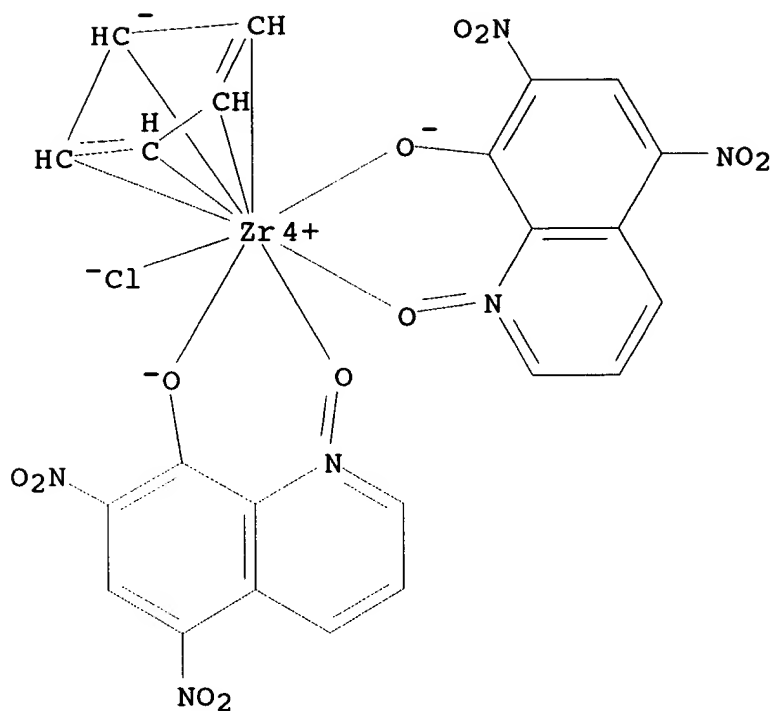


RN 98606-22-5 HCA  
 CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5-nitro-8-quinolinol 1-oxidato-O1,08)- (9CI) (CA INDEX NAME)



RN 98606-31-6 HCA  
 CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dinitro-8-quinolinol 1-oxidato-O1,08)- (9CI) (CA INDEX NAME)





CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 98606-19-0P 98606-20-3P 98606-21-4P

98606-22-5P 98606-31-6P

(prepn. and spectra of)

L38 ANSWER 9 OF 48 HCA COPYRIGHT 1998 ACS

102:105073 Chelated titanium(IV) derivatives of 1,1-diphenylethanol and phenolphthalein. Deshpande, S. S.; Awasarkar, P. A.; Gopinathan, Sarada; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Pune, 411 008, India). Indian J. Chem., Sect. A, 23A(11), 957-8 (English) 1984. CODEN: IJCADU. ISSN: 0376-4710.

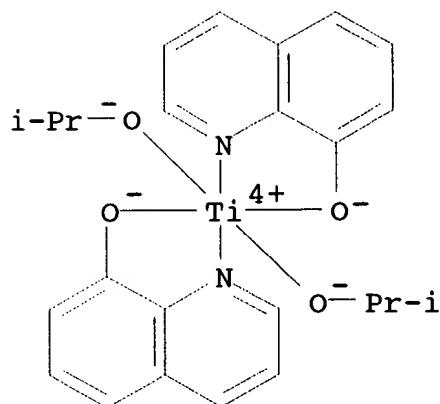
AB TiL2L12 (HL = (C6H5)2C(CH3)OH, HL1 = salicylaldehyde (I), 8-hydroxyquinoline (II), 2-hydroxyacetophenone, 2-hydroxy-4-methoxybenzophenone, BzN(Ph)OH, acetoacetanilide), TiL2L32 (H2L2 = phenolphthalein,; HL3 = I, II, Me salicylate, acetylacetone, benzoylacetone, dibenzoylmethane, BzN(Ph)OH), and (C5H5)2TiL2 (C5H5 = cyclopentadienyl) were prepd. from TiL12(OPr-iso)2 and HL or TiL32(OPr-iso)2 with H2L2, resp. The structures of the complexes were assigned on the basis of IR and 1H NMR spectral data. The complexes are monomeric and have an octahedral structure.

IT 23329-69-3

(reactions of, with diphenylethanol and phenolphthalein)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



QD411.J6

CC 78-7 (Inorganic Chemicals and Reactions)

IT 23329-69-3 59368-50-2 59368-51-3

(reactions of, with diphenylethanol and phenolphthalein)

L38 ANSWER 10 OF 48 HCA COPYRIGHT 1998 ACS

101:230699 Synthesis and properties of monocyclopentadienyltitanium compounds. Martin-Benito, R.; Jimenez-Aparicio, R.; Barral, M. C. (Fac. Cienc. Quím., Univ. Complut. Madrid, Madrid, Spain). J. Organomet. Chem., 269(3), 267-72 (English) 1984, CODEN: JORCAI. ISSN: 0022-328X.

AB The pentacoordinated complexes (RCp)TiCl<sub>2</sub>(acac) (R = H, Me, Ph<sub>2</sub>CH; RCp = R-substituted cyclopentadienyl, acac = acetylacetonate) were prepd. by photolysis of (RCp)<sub>2</sub>TiCl<sub>2</sub> and acacH in THF and the hexacoordinated compds. (RCp)TiCl(acac)<sub>2</sub> by the reaction of (RCp)<sub>2</sub>TiCl<sub>2</sub> and acacH in the presence of Et<sub>3</sub>N in isobutyronitrile. The hexacoordinated complexes (RCp)TiClL<sub>2</sub> (R = H, Me, Ph<sub>2</sub>CH; L = 8-oxyquinolate) were prepd. by the direct interaction of (RCp)<sub>2</sub>TiCl<sub>2</sub> and 8-hydroxyquinoline in isobutyronitrile; these compds. can be obtained more quickly by photolysis of the same starting materials in THF soln.

IT 93347-14-9P 93364-87-5P

(prepn. and cond. of)

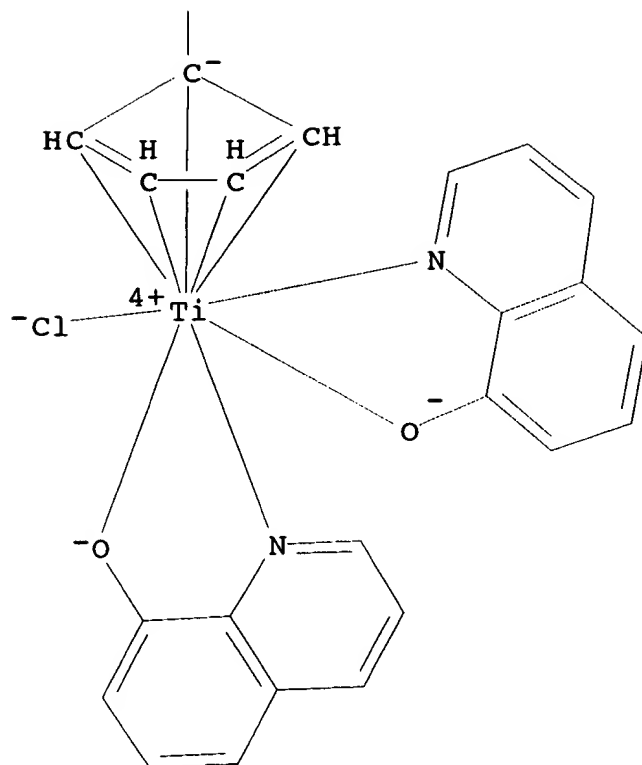
RN 93347-14-9 HCA

CN Titanium, chloro[(1,2,3,4,5-.eta.)-1-methyl-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

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Me  
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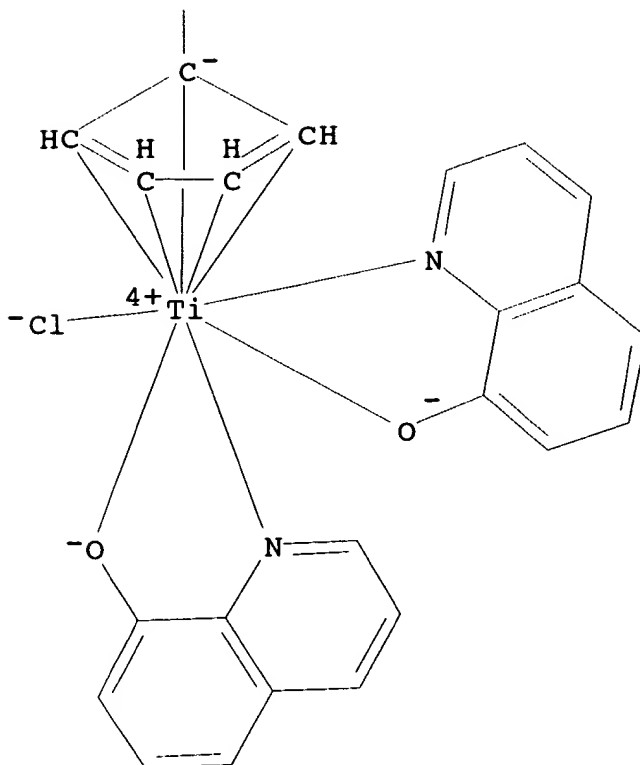


RN 93364-87-5 HCA  
 CN Titanium, chloro[(1,2,3,4,5-.eta.)-1-(diphenylmethyl)-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

PAGE 1-A

CHPh<sub>2</sub>  
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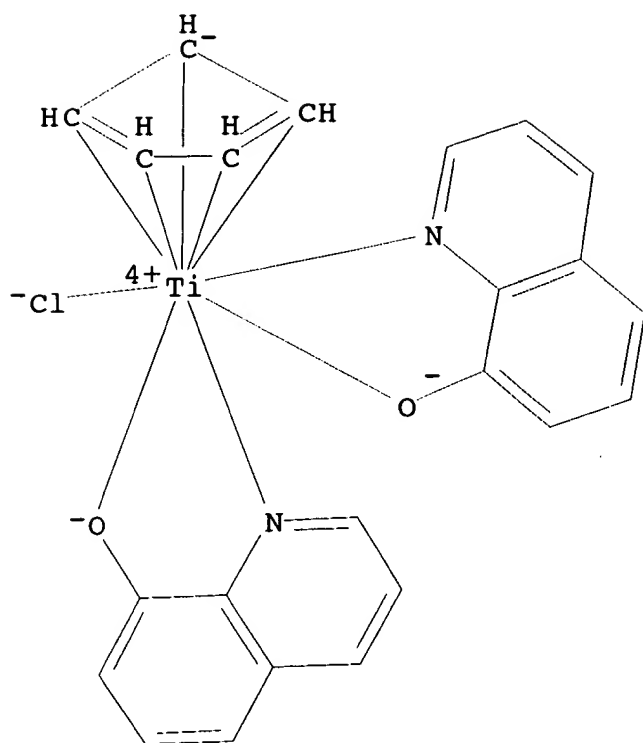


IT 31798-62-6P

(prepn. of)

RN 31798-62-6 HCA

CN Titanium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 93346-96-4P 93347-11-6P 93347-12-7P 93347-13-8P

93347-14-9P 93364-87-5P 93364-88-6P

(prepn. and cond. of)

IT 31798-62-6P

(prepn. of)

L38 ANSWER 11 OF 48 HCA COPYRIGHT 1998 ACS

101:82965 New titanium(IV) chloroacetates. Awasarkar, P. A.; Gopinathan, Sarada, Mrs.; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Pune, 411 008, India). Indian J. Chem., Sect. A, 22A(12), 1076-7 (English) 1983. CODEN: IJCADU. ISSN: 0376-4710.

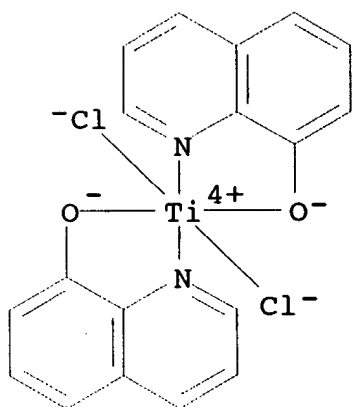
AB TiL2L12 (HL = ClCH2CO2H, HL1 = cyclopentadiene (HCp), acetylacetone (Hacac); HL = Cl2CHCO2H, HL1 = HCp, Hacac, salicylaldehyde, 2-hydroxyacetophenone, 8-hydroxyquinoline; HL = Cl3CCO2H, HL1 = HCp, salicylaldehyde) and Ti(O2CCCl3)4 were prep'd. from TiL12Cl2 and NaL. In TiL2L12 (HL1 .noteq. HCp), the acetate groups are monodentate to form octahedral complexes. No evidence for the assocn. of the mol. was obtained. In TiCp2L2, the acetate groups are bidentate.

IT 16905-40-1

(reaction of, with dichloroacetic acid)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
(CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 29

IT 16905-40-1 91408-55-8

(reaction of, with dichloroacetic acid)

L38 ANSWER 12 OF 48 HCA COPYRIGHT 1998 ACS

99:175962 Some reactions of 8-quinolinol N-oxide with bis(.eta.5-cyclopentadienyl)titanium dichloride. Goyal, K. C.; Khosla, B. D. (Dep. Chem., Univ. Delhi, Delhi, 110 007, India). J. Indian Chem. Soc., 60(4), 399-400 (English) 1983. CODEN: JICSAH. ISSN: 0019-4522.

AB Treating a mixt. of (.epsilon.5-C5H5)2TiCl2 (I) and 8-quinolinol N-oxide (II) with NaNH2 in PhMe under reflux gave (.epsilon.5-C5H5)2TiLCl (L = N-oxido-8-quinolinolato). Treating a mixt. of I and II in MeCN with Et3N gave (.epsilon.5-C5H5)2TiL2 (same L).

IT 87612-44-0P

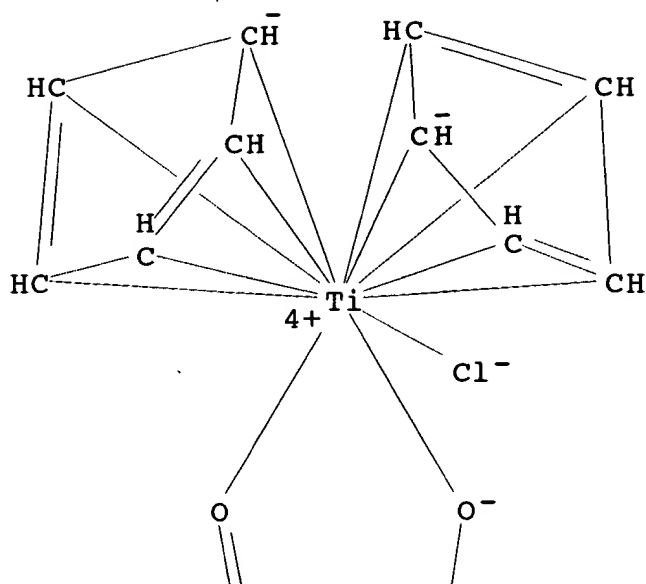
(prepn. of)

RN 87612-44-0 HCA

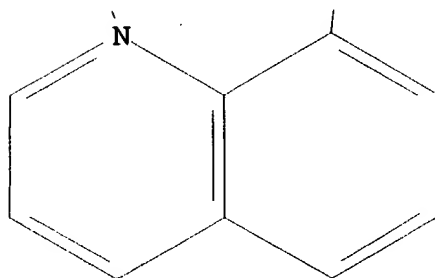
CN Titanium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinol 1-oxidato-O,O')- (9CI) (CA INDEX NAME)



PAGE 1-A



PAGE 2-A



CC 29-10 (Organometallic and Organometalloidal Compounds)  
 IT 87612-44-0P 87612-45-1P  
 (prepn. of)

L38 ANSWER 13 OF 48 HCA COPYRIGHT 1998 ACS  
 99:63207 Titanium(IV) and tin(IV) derivatives of salicylaldehyde  
 hydrazone and 2-hydroxyacetophenone hydrazone. Pardhy, Mrs. S. A.;

Gopinathan, Mrs. Sarada; Gopinathan, C. (Natl. Chem. Lab., Poona City, 411008, India). Synth. React. Inorg. Met.-Org. Chem., 13(4), 385-95 (English) 1983. CODEN: SRIMCN. ISSN: 0094-5714.

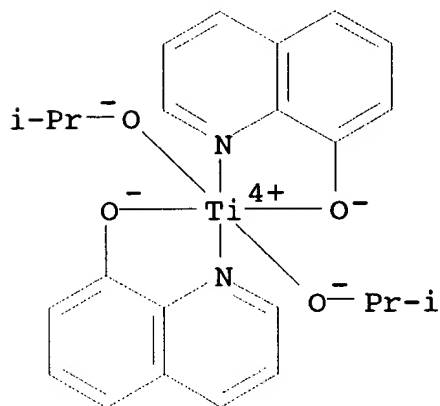
AB cis-R<sub>2</sub>SnL<sub>2</sub> (HL = salicylaldehyde hydrazone (HSA), 2-hydroxyacetophenone hydrazone (HAcPA); R = Me, Bu, octyl) and Ph<sub>3</sub>SnL were prepd. from R<sub>2</sub>SnCl<sub>2</sub> or Ph<sub>3</sub>SnCl, resp., and NaL. trans-TiL<sub>2</sub>Cl<sub>2</sub> were prepd. from TiCl<sub>4</sub> and HL. TiQ<sub>2</sub>(OPr-iso)<sub>2</sub> (HQ = 8-hydroxyquinoline) and iso-Pr titanate reacted with HL to give TiL<sub>2</sub>Q<sub>2</sub> and [TiL<sub>2</sub>O]<sub>2</sub>, resp. TiL<sub>12</sub>(OPr-iso)<sub>2</sub> (HL' = salicylaldehyde) or TiL<sub>22</sub>(OPr-iso)<sub>2</sub> (HL<sub>2</sub> = acetylacetone, benzoylacetone, dibenzoylmethane) reacted with HSA or HAcPA to give TiL<sub>32</sub> (H<sub>2</sub>L<sub>3</sub> = Schiff bases derived from HSA or HAcPA and HL<sub>1</sub> or HL<sub>2</sub>). These complexes were characterized by IR spectra.

IT 23329-69-3

(reaction of, with hydroxyacetophenone hydrazone and salicylaldehyde hydrazone)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 29

IT 12103-39-8 17927-72-9 23329-69-3 59368-51-3  
72439-63-5

(reaction of, with hydroxyacetophenone hydrazone and salicylaldehyde hydrazone)

L38 ANSWER 14 OF 48 HCA COPYRIGHT 1998 ACS

98:226899 Complexes of 8-quinolinol N-oxide with zirconium tetrachloride. Mittal, I. P.; Goyal, K. C.; Kaushik, N. K. (Dep. Chem., Univ. Delhi, Delhi, 110007, India). J. Inst. Chem. (India), 55(1), 29-32 (English) 1983. CODEN: JOICA7. ISSN: 0020-3254.

AB ZrCl<sub>4</sub>.2HL and ZrOCl<sub>2</sub>.2HL (HL = 8-quinolinol N-oxide) were prepd. from ZrCl<sub>4</sub> and HL in ether or EtOH, resp. When a 1:2 ZrCl<sub>4</sub>-HL mixt. was refluxed in C<sub>6</sub>H<sub>6</sub>, ZrCl<sub>2</sub>L<sub>2</sub> was obtained. ZrCl<sub>4</sub>.2HL and ZrCl<sub>2</sub>L<sub>2</sub>

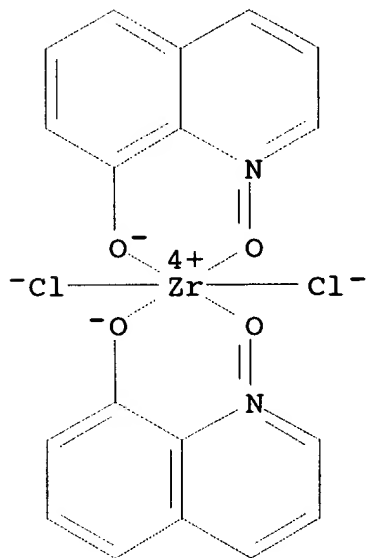
are 6-coordinate and  $\text{ZrOCl}_2 \cdot 2\text{HL}$  is 5-coordinate. In  $\text{ZrCl}_4 \cdot 2\text{HL}$  and  $\text{ZrOCl}_2 \cdot 2\text{HL}$ , HL is monodentate and coordinate through the N-O group.  $\text{ZrCl}_4 \cdot 2\text{HL}$  and  $\text{ZrOCl}_2 \cdot 2\text{HL}$  were characterized by thermogravimetry and IR spectra.

IT 85786-21-6P

(prepn. and IR spectrum of)

RN 85786-21-6 HCA

CN Zirconium, dichlorobis(8-quinolinol 1-oxidato-O,O')- (9CI) (CA INDEX NAME)



IT 85786-14-7P 85886-72-2P

(prepn., IR spectrum and thermogravimetry of)

RN 85786-14-7 HCA

CN Zirconium, dichlorooxobis(8-quinolinol 1-oxide-O,O')- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 85886-72-2 HCA

CN Zirconium, tetrachlorobis(8-quinolinol 1-oxide-O,O')- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

CC 78-7 (Inorganic Chemicals and Reactions)

IT 85786-21-6P

(prepn. and IR spectrum of)

IT 85786-14-7P 85886-72-2P

(prepn., IR spectrum and thermogravimetry of)

L38 ANSWER 15 OF 48 HCA COPYRIGHT 1998 ACS

98:34674 Organoxytitanium(IV) and organotin(IV) derivatives of

saligenin. Pandit, S. K.; Gopinathan, Sarada; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Poona City, 411 008, India). Indian J. Chem., Sect. A, 21A(7), 726-7 (English) 1982. CODEN: IJCADU. ISSN: 0376-4710.

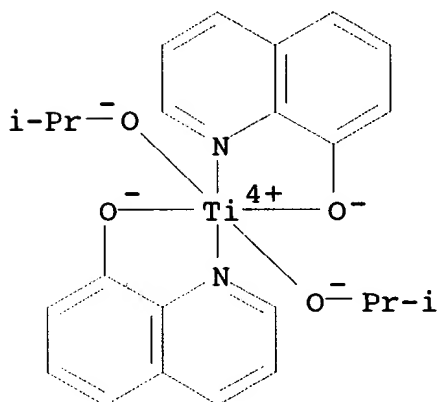
AB Disodiosaligenin reacts with  $\text{SnCl}_4$  giving a dichloride; with diorganotin dichlorides, it forms diorganostannylsaligenin derivs. IR and NMR spectra indicate that the Ti compds., prepd. from bischelated diisopropoxytitaniums and saligenin, are 6-coordinate, while the Sn derivs. are 4-coordinate.

IT 23329-69-3

(reaction of, with saligenin)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 12103-39-8 17927-72-9 23329-69-3 59368-50-2  
59368-51-3

(reaction of, with saligenin)

L38 ANSWER 16 OF 48 HCA COPYRIGHT 1998 ACS

95:72372 Complexes of titanium tetrachloride with 8-quinolinol N-oxide. Goyal, K. C.; Khosla, B. D. (Dep. Chem., Univ. Delhi, Delhi, 110 007, India). J. Indian Chem. Soc., 58(6), 617-19 (English) 1981. CODEN: JICSAH. ISSN: 0019-4522.

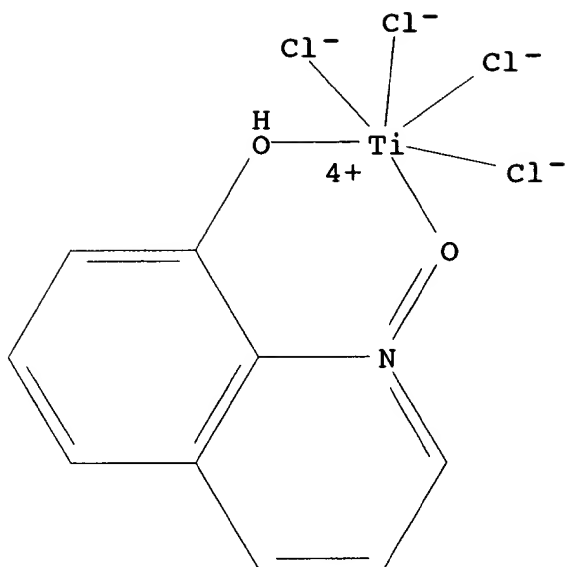
AB 8-Quinolinol N-oxide (HL) reacts with  $\text{TiCl}_4$  to give  $\text{TiCl}_4 \cdot \text{HL}$  and  $\text{TiCl}_4 \cdot 2\text{HL}$ . Both adducts undergo thermal decompn. to give  $\text{TiCl}_2\text{L}_2$  and finally  $\text{TiO}_2$ . The complexes were characterized by chem. anal. and IR spectra. The IR spectra indicate that HL acts as a bidentate ligand in these complexes.

IT 78505-44-9P 78505-45-0P 78505-46-1P

(prepn. and thermal decompn. of)

RN 78505-44-9 HCA

CN Titanium, tetrachloro(8-quinolinol 1-oxide-O,O')-, (OC-6-32)- (9CI) (CA INDEX NAME)

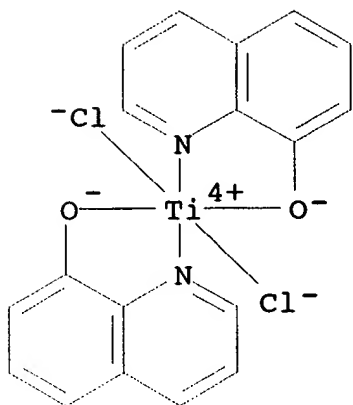


RN 78505-45-0 HCA  
 CN Titanium, tetrachlorobis(8-quinolinol 1-oxide-O,O')- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 78505-46-1 HCA  
 CC 78-7 (Inorganic Chemicals and Reactions)  
 IT 78505-44-9P 78505-45-0P 78505-46-1P  
 (prepn. and thermal decompn. of)

L38 ANSWER 17 OF 48 HCA COPYRIGHT 1998 ACS  
 94:113628 The isolation and characterization of some mixed ligand complexes of titanium(IV). Aly, Mohamed M.; Hassan, Mostafa K. (Fac. Sci., Assiut Univ., Assiut, Egypt). Ann. Chim. (Rome), 70(9-10), 463-70 (English) 1980. CODEN: ANCRAI. ISSN: 0003-4592.  
 AB  $TiCl_4(HL)_2$  (I; HL = 8-quinolinol) reacts with acetylacetone or salicylaldehyde to give  $TiCl_2L_2$ . I reacts with  $CF_3CO_2H$  to give  $Ti(O_2CCF_3)_2L_2$  and with other haloacetates to give  $TiClL'L_2$  (HL' =  $CCl_3CO_2H$ ,  $CHCl_2CO_2H$ ). I and pyridine-2,6-dicarboxylic acid ( $H_2L''$ ) give  $TiCl(HL'')L_2.HCl$ . A coordination no. of 8 is proposed for the  $TiClL'L_2$  and  $TiCl(HL'')L_2.HCl$  complexes with Cl bridging ligands and bidentate L, L' and HL'' ligands.  
 IT 16905-40-1P 76770-41-7P 76770-43-9P  
 76779-21-0P  
 (prepn. of)  
 RN 16905-40-1 HCA  
 CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

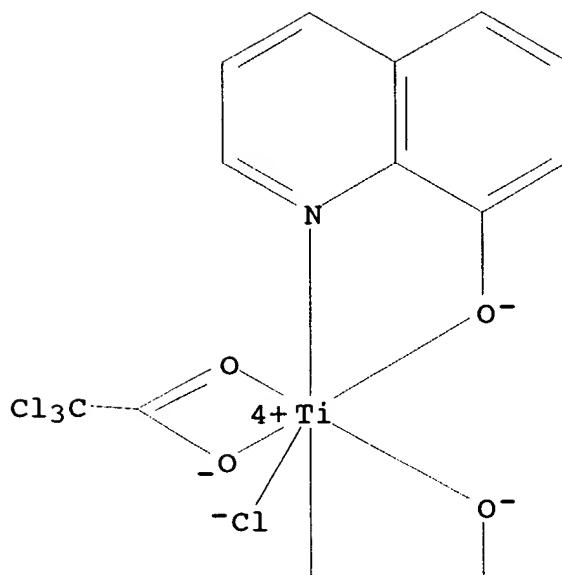


RN 76770-41-7 HCA  
CN Titanium, chlorobis(8-quinolinolato-N1,O8)(trichloroacetato-O,O')-,  
homopolymer (9CI) (CA INDEX NAME)

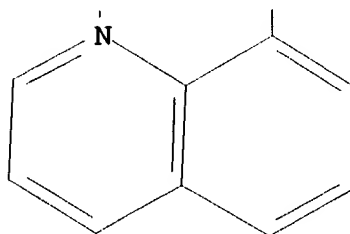
CM 1

CRN 76770-40-6  
CMF C20 H12 Cl4 N2 O4 Ti  
CCI CCS

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PAGE 2-A

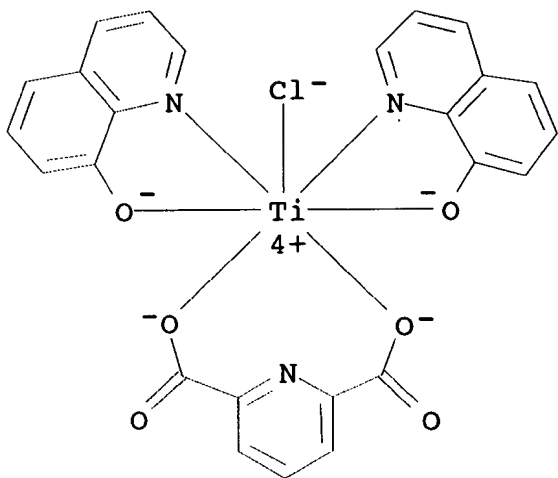


RN 76770-43-9 HCA  
 CN Titanium, chloro[2,6-pyridinedicarboxylato(2-)-O2,O6]bis(8-quinolinolato-N1,08)-, monohydrochloride, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 76770-42-8

CMF C25 H15 Cl N3 O6 Ti . Cl H  
CCI CCS



● HCl

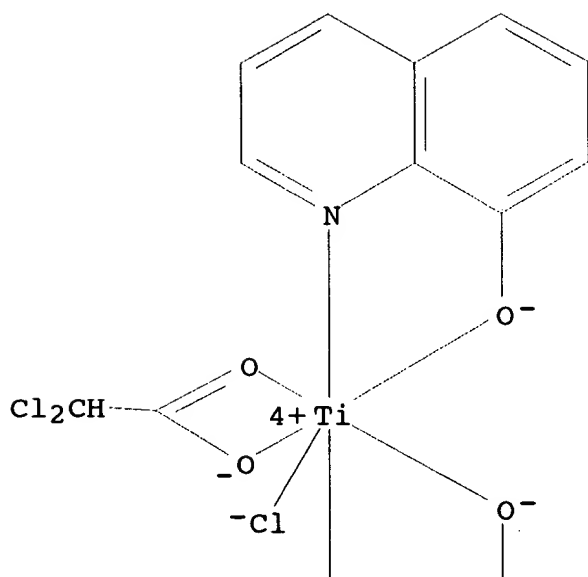
RN 76779-21-0 HCA  
CN Titanium, chloro(dichloroacetato-O,O')bis(8-quinolinolato-N1,O8)-,  
homopolymer (9CI) (CA INDEX NAME)

CM 1

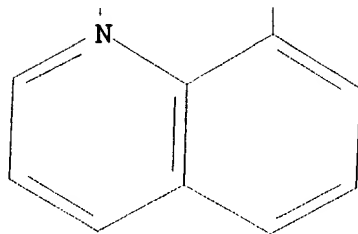
CRN 76779-20-9  
CMF C20 H13 Cl3 N2 O4 Ti  
CCI CCS



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PAGE 2-A



CC 78-7 (Inorganic Chemicals and Reactions)  
 IT 16905-40-1P 76770-41-7P 76770-43-9P  
 76771-15-8P 76779-21-0P  
 (prepn. of)

L38 ANSWER 18 OF 48 HCA COPYRIGHT 1998 ACS  
 94:15831 Bis-chelated titanium(IV) derivatives of triphenylsilanol,  
 diphenylsilanediol and triphenylcarbinol. Unny, I. R.; Gopinathan,

Sarada; Gopinathan, C. (Natl. Chem. Lab., Poona City, 411 008, India). Indian J. Chem., Sect. A, 19A(6), 598-9 (English) 1980. CODEN: IJCADU. ISSN: 0376-4710.

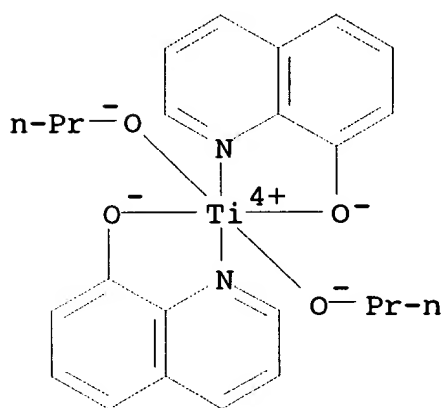
AB Bis-chelated Ti(IV) diisopropoxides,  $L_2Ti(OPr)_2$ , react with triphenylsilanol, diphenylsilanediol and triphenylcarbinol giving products  $L_2Ti(OSiPh_3)_2$ ,  $L_2Ti(O_2SiPh_2)$  and  $L_2Ti(OCPh_3)_2$  resp. The ligands (L) used are salicylaldehyde, acetylacetone, 8-hydroxyquinoline, acetoacetanilide and 2-hydroxy-4-methoxybenzophenone.  $Ti(OPr)_4$  reacts with triphenylcarbinol giving  $Ti(OCPh_3)_4$ . The new titanosiloxanes have good thermal stabilities.

IT 75576-95-3

(reaction of, with alcs.)

RN 75576-95-3 HCA

CN Titanium, dipropoxybis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 3087-37-4 21474-51-1 50363-05-8 75576-94-2 75576-95-3  
75576-96-4

(reaction of, with alcs.)

L38 ANSWER 19 OF 48 HCA COPYRIGHT 1998 ACS

92:198492 Bromides and phenoxides of bis(cyclopentadienyl)chelate derivatives of zirconium. Brainina, E. M.; Minacheva, M. Kh. (Inst. Elementoorg. Soedin., Moscow, USSR). Izv. Akad. Nauk SSSR, Ser. Khim. (2), 410-13 (Russian) 1980. CODEN: IASKA6. ISSN: 0002-3353.

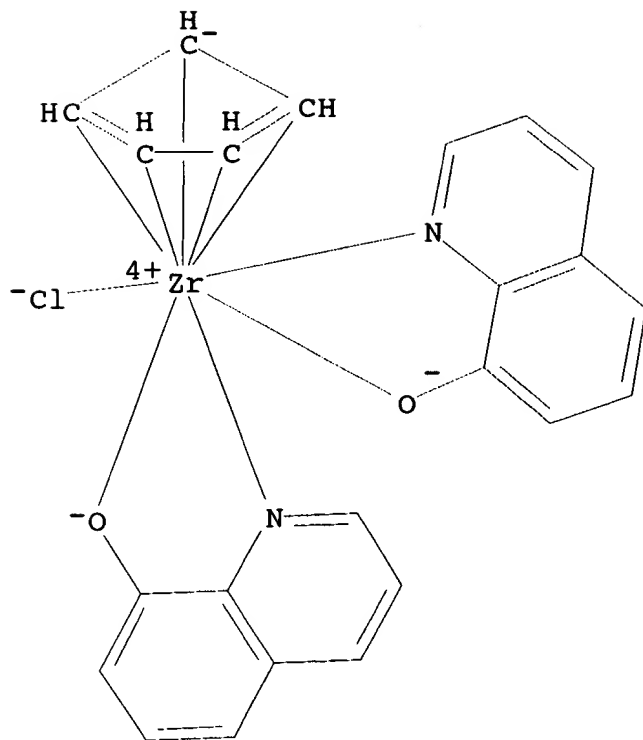
AB (.eta.5-C5H5)2ZrLX (LH = BzCH2Ac, Bz2CH2, (L1H), 8-hydroxyquinoline; X = Br, PhO) were prepd. in 41-81% yields. Thus, treating [(eta.5-C5H5)2ZrBr]2O with L1H gave 44% (.eta.5-C5H5)2ZrL1Br.cntdot.H2O.

IT 12114-15-7P 73655-94-4P

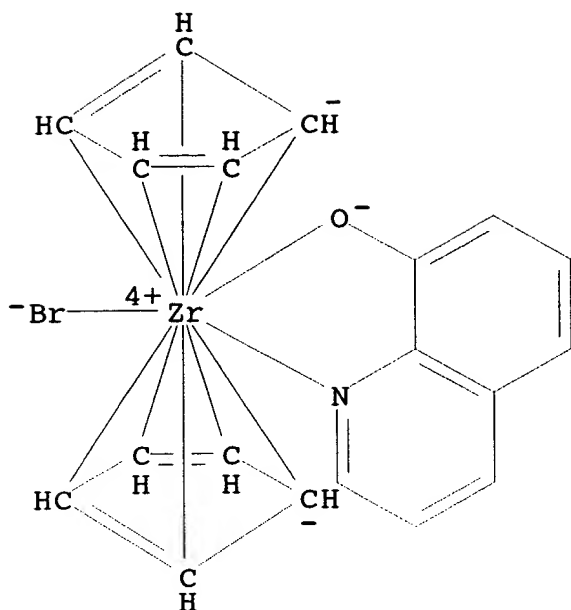
(prepn. of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



RN 73655-94-4 HCA  
CN Zirconium, bromobis(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-  
N1,O8)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT **12114-15-7P** 39475-31-5P 73655-93-3P **73655-94-4P**  
 73655-95-5P 73655-96-6P 73655-97-7P 73655-98-8P 73655-99-9P  
 73667-87-5P  
 (prepn. of)

L38 ANSWER 20 OF 48 HCA COPYRIGHT 1998 ACS

92:76627 The reactions of tert-butyl isocyanide with halides of titanium(IV), hafnium(IV), vanadium(III), niobium(IV), molybdenum(V) and tungsten(VI); insertion into metal-halogen bonds and ligand displacement reactions. Behnam-Dehkordy, Mahbobeh; Crociani, Bruno; Nicolini, Marino; Richards, Raymond L. (Sch. Mol. Sci., Univ. Sussex, Brighton, BN1 9QJ, Engl.). J. Organomet. Chem., 181(1), 69-80 (English) 1979. CODEN: JORCAI. ISSN: 0022-328X.

AB t-BuNC inserts into a metal-halogen bond of  $\text{TiCl}_4$ ,  $\text{HfCl}_4$ ,  $\text{VCl}_3$  and  $[\text{NbCl}_4(\text{THF})_2]$  to give  $[\text{TiCl}_3\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{CNBu-t})]_2$ ,  $[\text{HfCl}_3\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{CNBu-t})]_2$ ,  $[\text{VCl}_2\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{CNBu-t})]_2$  and  $[\text{NbCl}_3\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{CNBu-t})]_2$ , resp.  $[\text{MoCl}_4(\text{THF})_2]$  and  $\text{WCl}_6$  do not give inserted products, but rather  $[\text{MoCl}_3(\text{CNBu-t})_3]\text{Cl}$  and  $\text{trans-}[\text{WCl}_4(\text{CNBu-t})_2]$ . Treatment of these inserted products and  $[\text{MX}_4\{\text{C}(\text{X})\text{NBu-t}\}(\text{CNBu-t})]_2$  ( $\text{M} = \text{Nb}$  or  $\text{Ta}$ ,  $\text{X} = \text{Cl}$  or  $\text{Br}$ ) with Li quinolin-8-olate ( $\text{Li}[8\text{-quin}]$ ), Na diethyldithiocarbamate ( $\text{Na}[\text{dtc}]$ ) or  $\text{Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2$  (dppe) causes displacement of terminal t-BuNC in all cases and in some cases of the iminoethyl ligand as well. Thus obtained are the complexes  $[\text{TiCl}_2\{\text{C}(\text{Cl})\text{NBu-t}\}(8\text{-quin})]$ ,  $[\text{TiCl}_4(\text{dppe})]$ ,  $[\text{TiCl}_2(\text{dtc})_2]$ ,  $[\text{HfCl}_2\{\text{C}(\text{Cl})\text{NBu-t}\}(8\text{-quin})]$ ,  $[\text{HfCl}_3\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{dppe})]$ ,  $[\text{Hf}(\text{dtc})_4]$ ,  $[\text{VCl}\{\text{C}(\text{Cl})\text{NBu-t}\}(8\text{-quin})]$ ,  $[\text{V}(\text{dtc})_4]$ ,  $[\text{NbCl}_2\{\text{C}(\text{Cl})\text{NBu-t}\}(8\text{-quin})]_2$ ,  $[\text{NbCl}\{\text{C}(\text{Cl})\text{NBu-t}\}(\text{dtc})]_2$ ,  $[\text{MX}_3\{\text{C}(\text{X})\text{NBu-t}\}(8\text{-quin})]$  ( $\text{M} = \text{Nb}$  or  $\text{Ta}$ ,  $\text{X} = \text{Cl}$  or  $\text{Br}$ ),

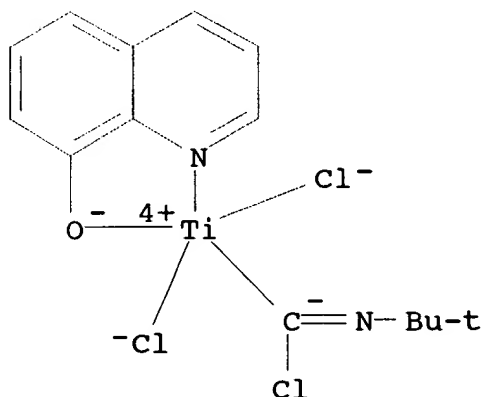
$[\text{NbX}_2\{\text{C}(\text{X})\text{NBu-t}\}(\text{dtc})_2]$  and  $[\text{TaX}_3\{\text{C}(\text{X})\text{NBu-t}\}(\text{dtc})]_2$ .  $\text{Ta}_2\text{Br}_{10}$  gives  $\text{TaB}_3(\text{dtc})_2$  on treatment with  $\text{Na}[\text{dtc}]$ .

IT 72637-85-5P 72637-86-6P

(prepn. and spectral properties of)

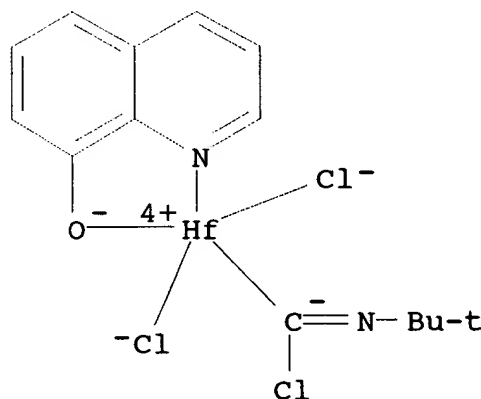
RN 72637-85-5 HCA

CN Titanium, dichloro[chloro[(1,1-dimethylethyl)imino]methyl](8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



RN 72637-86-6 HCA

CN Hafnium, dichloro[chloro[(1,1-dimethylethyl)imino]methyl](8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

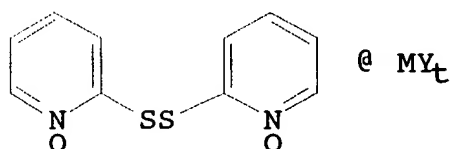
IT	12406-70-1P	57974-86-4P	57974-88-6P	57974-90-0P	58019-14-0P
	71737-46-7P	72637-85-5P	72637-86-6P		
	72637-87-7P	72637-88-8P	72637-89-9P	72637-90-2P	72637-93-5P
	72637-94-6P	72637-95-7P	72637-96-8P	72637-98-0P	72638-00-7P
	72638-01-8P				

(prepn. and spectral properties of)

L38 ANSWER 21 OF 48 HCA COPYRIGHT 1998 ACS

91:163068 Synergistic compositions and method of use to treat inflammation. Klein, Robert W.; Nuss, George W., Jr. (USA). U.S. US 4163783 790807, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 77-835595 770922.

GI



AB A synergistic topical inflammation inhibiting compn. contains a nonsteroid inflammation inhibitor and I (M = Zn, Fe, Mg, Sn, Cd, Zr, or alkali and alk. earth metals; Y = anion; t = 1 or 2). A topical cream (100 g) was prepd. contg. I (M = Ca, Y = Cl, t = 2) [43143-10-8] 1 g and 1-(p-chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid [53-86-1] 0.3 g.

IT 70675-90-0

(synergistic topical inflammation inhibiting compns. contg.)

RN 70675-90-0 HCA

CN Zirconium, tetrachloro[2,2'-dithiobis[pyridine] 1,1'-dioxide-O,O',S]- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IC A61K031-44; A61K031-555

NCL 424245000

CC 63-6 (Pharmaceuticals)

IT 43143-10-8 70675-89-7 70675-90-0 70675-91-1

70848-99-6 70849-00-2 70849-02-4 71724-05-5

(synergistic topical inflammation inhibiting compns. contg.)

L38 ANSWER 22 OF 48 HCA COPYRIGHT 1998 ACS

91:97345 Configurational rearrangements in cis-M(AA)2X2, cis-M(AA)2XY, and cis-M(AB)2X2 complexes. 6. Bis(chelate)bis(2,6-diisopropylphenoxy)titanium systems (chelate = acetylacetonate, 8-hydroxyquinolate, and 8-hydroxyquinaldinate). Bickley, Douglas G.; Serpone, Nick (Dep. Chem., Concordia Univ., Montreal, PQ, H3G 1M8, Can.). Inorg. Chem., 18(8), 2200-4 (English) 1979. CODEN: INOCAJ. ISSN: 0020-1669.

AB For a series of bis(chelate), bis(2,6-diisopropylphenoxy)titanium complexes [chelate = acetylacetonate (acac), 8-hydroxyquinolate (ox), and 8-hydroxyquininate (quin)] an NMR total line shape anal. of iso-Pr Me group exchange (inversion) is reported, along with data for acac Me group exchange for the corresponding acac complex. Activation energies (kcal/mol) and entropies (entropy units), in

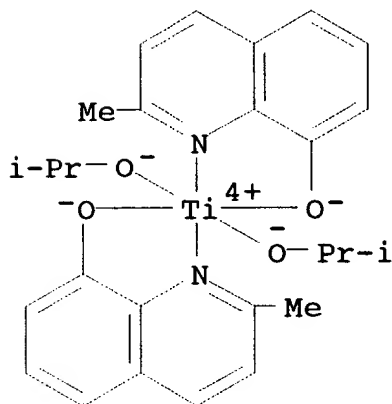
m-dichlorobenzene solns., for inversion are, resp., 6.3  $\pm$  1.7 and -36.5  $\pm$  5.7 (acac), 14.7  $\pm$  0.8 and -9.7  $\pm$  2.2 (quin), and 21.2  $\pm$  1.3 and 2.2  $\pm$  3.3 (ox). For acac Me group exchange, the corresponding kinetic data are (in m-dichlorobenzene soln.) 13.8  $\pm$  0.3 and -10.6  $\pm$  1.0. Dramatic differences between kinetic parameters suggest that the ox and quin complexes possess a different rearrangement route than that for the acac complex. On the assumption that the ox and quin complexes retain the same structure in solid and soln. phases, the iso-Pr Me group exchange is identified as resulting from the process  
 cis(phenoxy),cis(n),trans(O)-.DELTA.(.lambda.) .dblarw.  
 cis(phenoxy)cis(n),trans(O)-.lambda.(.DELTA.). This rearrangement stereochem. can only be generated via a Ti-n bond-rupture mechanism occurring through a trigonal-bipyramidal axial intermediate.

IT 33888-32-3P

(prepn. and substitution reaction of)

RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,O8)bis(2-propanolato)-(9CI) (CA INDEX NAME)



CC 67-3 (Catalysis and Reaction Kinetics)

Section cross-reference(s): 73

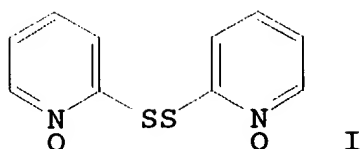
IT 33888-32-3P

(prepn. and substitution reaction of)

L38 ANSWER 23 OF 48 HCA COPYRIGHT 1998 ACS

91:78909 Compositions for treating inflammation. Klein, Robert W.  
 (Rorer, William H., Inc., USA). U.S. US 4152431 790501, 5 pp.  
 (English). CODEN: USXXAM. APPLICATION: US 77-835594 770922.

GI



AB Topical antiinflammatory compns. contain bis(2-pyridyl-1-oxide) disulfide (I) [3696-28-4] or I.MYt when M = Zn, Fe, Mg, Sn, Cd, Zr, or alkali or alk. earth metals and Y is an anion and t = 1 or 2. Topical compns. such as creams, ointments, or aerosols were prepd. contg. I derivs. such as I.MgSO<sub>4</sub> [70849-05-7] or I.CaCl<sub>2</sub> [70849-06-8].

IT **70849-04-6**

(inflammation inhibiting topical compns. contg.)

RN 70849-04-6 HCA

IC A61K031-44; A61K031-555

NCL 424245000

CC 63-6 (Pharmaceuticals)

IT 3696-28-4 70848-99-6 70849-00-2 70849-01-3 70849-02-4

70849-03-5 **70849-04-6** 70849-05-7 70849-06-8

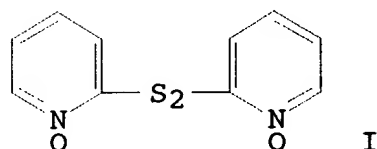
71016-06-3

(inflammation inhibiting topical compns. contg.)

L38 ANSWER 24 OF 48 HCA COPYRIGHT 1998 ACS

91:62729 Antiinflammatory agent. Klein, Robert Warren; Nuss, George Werner, Jr. (Rorer, William H., Inc., USA). Ger. Offen. DE 2840684 790405, 24 pp. (German). CODEN: GWXXBX. PRIORITY: US 77-835594 770922.

GI



AB A topical antiinflammatory compn. contains dithiobis(2-pyridine 1-oxide) (I) [3696-28-4] or a complex L<sub>2</sub>MX<sub>n</sub> (L = I; M = Zn, Fe, Mg, Sn, Cd, Zr, alkali metal, alk. earth metal; X = anion; n = 1, 2) and optionally another inflammation inhibitor. Thus an ointment was prepd. from I.CaCl<sub>2</sub> [70675-92-2] 2 and hydrocortisone (II) [50-23-7] 0.05 g. A mixt. of I.MgCl<sub>2</sub> [43143-11-9] 4 mg and II 1 mg caused 67.5% inhibition of croton oil-induced edema in mice.

IT **70675-90-0**

(topical antiinflammatory compn. contg.)



RN 70675-90-0 HCA  
CN Zirconium, tetrachloro[2,2'-dithiobis[pyridine] 1,1'-dioxide-O,O',S]-  
(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IC A61K031-44; A61K031-095; A61K031-57

CC 63-6 (Pharmaceuticals)

IT 3696-28-4 43143-11-9 70675-87-5 70675-88-6 70675-89-7

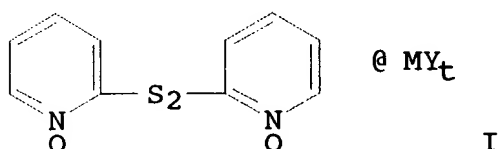
70675-90-0 70675-91-1 70675-92-2

(topical antiinflammatory compn. contg.)

L38 ANSWER 25 OF 48 HCA COPYRIGHT 1998 ACS

90:142170 Synergistic compositions. Klein, Robert W.; Nuss, George W., Jr. (Rorer, William H., Inc., USA). U.S. US 4137311 790130, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 77-835596 770922.

GI



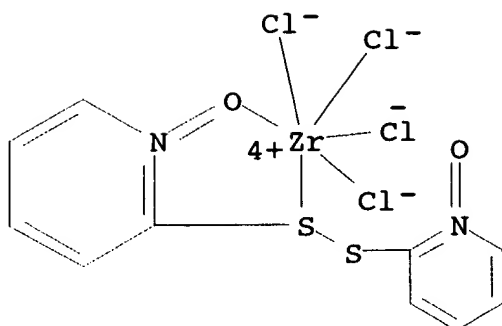
AB Antiinflammatory compns. for treating skin are prepd. comprising synergistic combination of a corticosteroid and bis(2-pyridyl-1-oxide) metal salts (I, M = metal, Y = anion, t = 1 or 2). Thus, an antiinflammatory dosage of 4 mg bis(2-pyridyl-1-oxide)disulfide magnesium sulfate [43143-11-9] and 1 mg hydrocortisone [50-23-7] produced 67.5% inhibition of croton oil-induced edema to mouse's ear. Dermatol. cleansing cakes and powders were prepd. contg. these synergistic mixts.

IT 69697-31-0

(antiinflammatory synergistic compns. contg. corticosteroids and)

RN 69697-31-0 HCA

CN Zirconium, tetrachloro[2,2'-dithiobis[pyridine] 1,1'-dioxide]-, (OC-6-33)- (9CI) (CA INDEX NAME)



IC A61K031-56

NCL 424240000

CC 63-6 (Pharmaceuticals)

IT 43143-10-8 43143-11-9 43143-12-0 69697-29-6 69697-30-9

69697-31-0 69697-32-1

(antiinflammatory synergistic compns. contg. corticosteroids and)

L38 ANSWER 26 OF 48 HCA COPYRIGHT 1998 ACS

90:33240 Studies on 8-quinolinol-N-oxides and some of their metal chelates. Ghuge, K. D.; Umapathy, P.; Sen, D. N. (Natl. Chem. Lab., Poona City, India). J. Indian Chem. Soc., 55(9), 864-8 (English) 1978. CODEN: JICSAH. ISSN: 0019-4522.

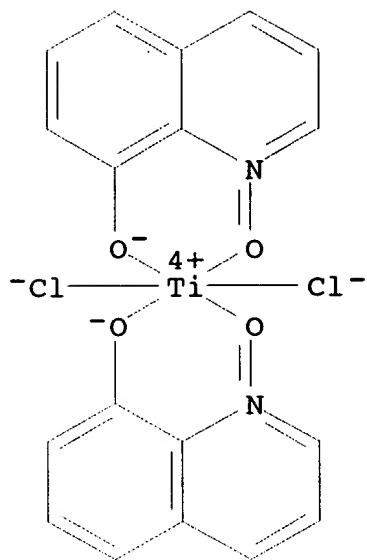
AB Several metal chelates of 8-quinolinol N-oxide with Cu(II), Be, Mn(II), Sn(II), Fe(III), Cr(III), Al, Sn(IV), Ti(IV), UO<sub>2</sub><sup>2+</sup>, VO<sub>2</sub><sup>+</sup> and MoO<sub>2</sub><sup>2+</sup> and also Cu(II), Fe(III), VO<sub>2</sub><sup>+</sup>, and VO<sub>2</sub><sup>2+</sup> chelates of 5-nitro-, 5,7-dinitro- and 5,7-dibromo-8-quinolinol N-oxide, were prepd. in pure state. These chelates are characterized by their elemental analyses, IR, UV-visible spectral, and magnetic susceptibility data wherever possible. The ligands act as bidentate, chelating agents, coordinating through the NO O and the phenolic hydroxyl O atoms. IR evidence is provided for the monodentate neutral character of the ligands in Sn(II) and Sn(IV) complexes. Deuteration studies were also made.

IT 68811-33-6P 68811-34-7P

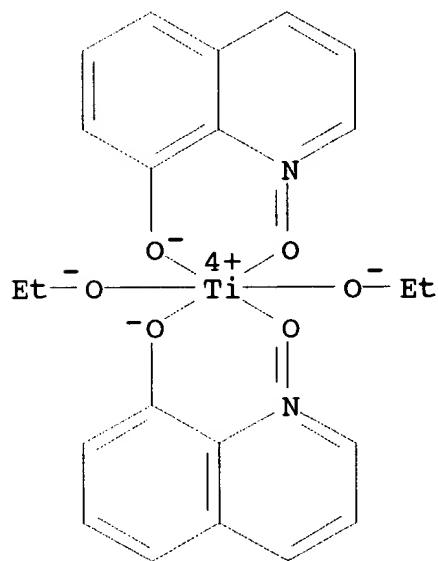
(prepn. of)

RN 68811-33-6 HCA

CN Titanium, dichlorobis(8-quinolinol 1-oxidato-O,O')- (9CI) (CA INDEX NAME)



RN 68811-34-7 HCA  
 CN Titanium, diethoxybis(8-quinolinol 1-oxidato-O,O')- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)  
 IT 52519-37-6P 52519-38-7P 68811-10-9P 68811-11-0P 68811-12-1P  
 68811-24-5P 68811-25-6P 68811-26-7P 68811-27-8P 68811-28-9P  
 68811-29-0P 68811-30-3P 68811-31-4P 68811-32-5P  
**68811-33-6P 68811-34-7P 68811-35-8P**

68811-36-9P 68811-37-OP 68824-12-4P  
(prepn. of)

L38 ANSWER 27 OF 48 HCA COPYRIGHT 1998 ACS

89:24870 Synthesis of polymers based on chelate titanium compounds.  
Nogaideli, A. I.; Mikhailov, M. B.; Pichkhadze, Sh. V. (Tbilis. Gos.  
Univ., Tiflis, USSR). Izv. Akad. Nauk Gruz. SSR, Ser. Khim., 3(4),  
344-9 (Russian) 1977. CODEN: IGSKDH.

AB Four copolymers were prepd. by polycondensation of  
bis(benzoylacetonato)bis(butanolato)titanium and  
bis(butanolato)bis(8-quinolinolato)titanium (I) with hydroquinone  
and 2,2-bis(4-hydroxyphenyl)propane (II). The reactions were  
conducted at 170.degree. and 1:1 molar ratio of the comonomers. The  
structure of the copolymers was established on the basis of  
evolution of BuOH during the polymn., elemental anal., and IR  
spectra. The red-brown copolymers were sol. in dioxane, DMF, and  
THF. The presence of I and II units in the copolymers shifted their  
glass transition to higher temps.

IT 66690-01-5P 66690-02-6P

(prepn., properties and structure of)

RN 66690-01-5 HCA

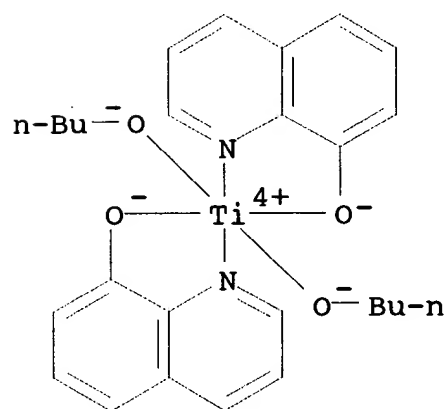
CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)-, polymer with  
1,4-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 17034-82-1

CMF C26 H30 N2 O4 Ti

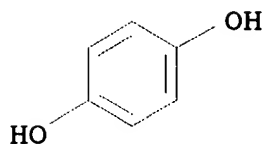
CCI CCS



CM 2

CRN 123-31-9

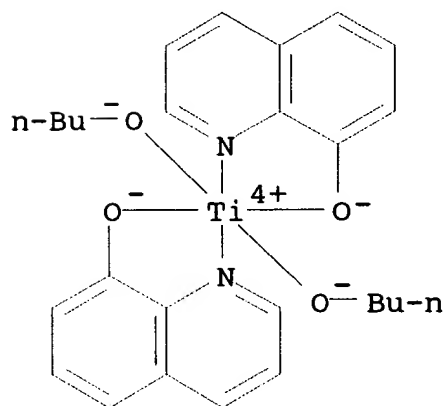
CMF C6 H6 O2



RN 66690-02-6 HCA  
 CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)-, polymer with  
 4,4'-(1-methylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

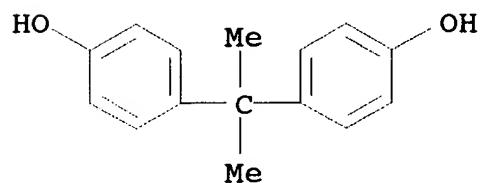
CM 1

CRN 17034-82-1  
 CMF C26 H30 N2 O4 Ti  
 CCI CCS



CM 2

CRN 80-05-7  
 CMF C15 H16 O2

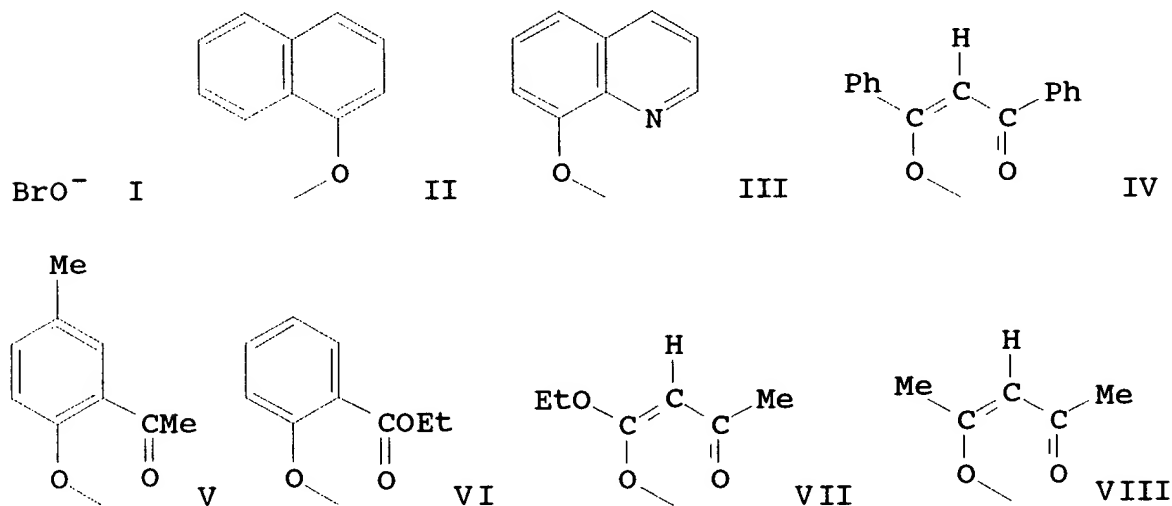


CC 35-3 (Synthetic High Polymers)

IT 66689-99-4P 66690-00-4P **66690-01-5P 66690-02-6P**  
 66690-04-8P 66690-06-0P 66690-08-2P 66690-10-6P  
 (prepn., properties and structure of)

L38 ANSWER 28 OF 48 HCA COPYRIGHT 1998 ACS  
 87:53910 Thermal stability of some chelate titanasiloxane oligomers.  
 Krivonishchenko, V. V.; Suvorov, A. L.; Malyarenko, A. V. (Inst.  
 Khim., Sverdlovsk, USSR). Vysokomol. Soedin., Ser. B, 19(5), 382-6  
 (Russian) 1977. CODEN: VYSBAI.

GI



AB The title polymers of structure  $\text{BuO}(\text{TiR}_2\text{OSiMe}_2\text{C}_6\text{H}_4\text{SiMe}_2\text{O})_n\text{H}$  (R = I-VIII) with coordinatively satd. Ti atoms in the main chain (R = III-VIII), in contrast to alkoxy- or aryloxytitanasiloxanes (R = I-II), were resistant to thermal disproportionation and their oxidative thermal stability was detd. by the structure of the chelated ligand at the Ti. The investigated polymers were prepd. by condensation of p-(HOSiMe<sub>2</sub>)C<sub>6</sub>H<sub>4</sub> with (BuO)<sub>2</sub>TiR<sub>2</sub>, and their stability was compared with that of oligomeric HO(TiR<sub>2</sub>O)<sub>n</sub>H (R = III-V, n = 2-3), modeling the chain units of the polymers.

IT **63533-38-0 63559-75-1**

(oxidative thermal stability of)

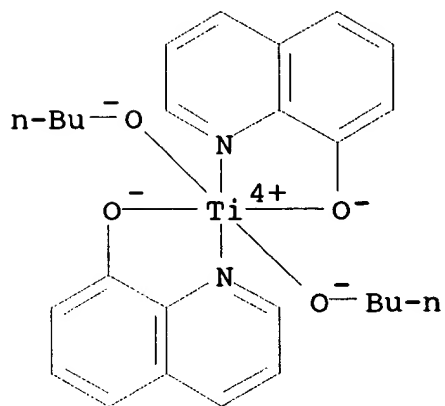
RN 63533-38-0 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)-, homopolymer (9CI)  
 (CA INDEX NAME)

CM 1

CRN 17034-82-1

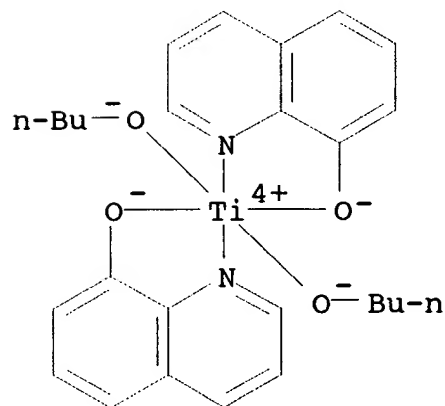
CMF C26 H30 N2 O4 Ti  
CCI CCS



RN 63559-75-1 HCA  
CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)-, polymer with  
1,4-phenylenebis[dimethylsilanol] (9CI) (CA INDEX NAME)

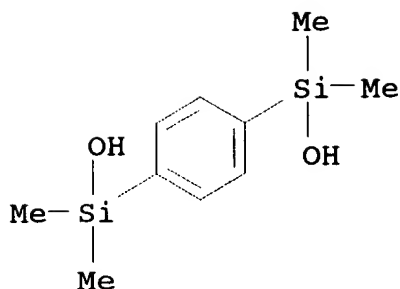
CM 1

CRN 17034-82-1  
CMF C26 H30 N2 O4 Ti  
CCI CCS



CM 2

CRN 2754-32-7  
CMF C10 H18 O2 Si2



CC 36-4 (Plastics Manufacture and Processing)  
 IT 63525-74-6 63525-76-8 63533-31-3 63533-33-5 63533-35-7  
 63533-36-8 63533-37-9 **63533-38-0** 63533-39-1  
**63559-75-1** 63587-27-9  
 (oxidative thermal stability of)

L38 ANSWER 29 OF 48 HCA COPYRIGHT 1998 ACS  
 84:74865 Polychelatotitanoarylenesiloxanes. Suvorov, A. L.; Malykhin, A. P.; Malyarenko, A. V. (Ural Institute of Chemistry, USSR). U.S.S.R. SU 492524 751125 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1975, 52(43), 64-5. (Russian). CODEN: URXXAF. APPLICATION: SU 73-1948565 730712.  
 AB The title compds. with improved thermal and oxidative stability were prep'd. by polycondensing an unsat'd. bis(chelato)dialkoxytitanium, e.g. bis(7-allyl-8-quinolyloxy)dibutoxytitanium [58249-06-2], bis(2-methacryloyl-4-methylphenoxy)dibutoxytitanium [58218-70-5], bis(2-allyl-6-carbethoxyphenoxy)diethoxytitanium [58218-71-6], or bis(2-carballyloxyphenoxy)diethoxytitanium [58218-72-7] with arom. bis(hydroxydiorganosilyl) compds. at 40-80.degree. in Et2O [60-29-7] as the solvent.  
 IC C08G  
 CC 35-3 (Synthetic High Polymers)

L38 ANSWER 30 OF 48 HCA COPYRIGHT 1998 ACS  
 84:68867 Chemistry of phenoxo complexes. III. Preparation and characterization of some bis(chelato)bis(phenoxo)titanium(IV) complexes. Harrod, J. F.; Taylor, K. R. (Chem. Dep., McGill Univ., Montreal, Que., Can.). Inorg. Chem., 14(7), 1541-5 (Enlis) 195. CODEN: INOCAJ.  
 AB A large no. of bis(chelato)bis(phenoxo)titanium(IV) complexes were prep'd. by metathesis between a phenol and bis(chelato)bis(alkoxo)titanium(IV), where chelato = acetylacetonato, 8-quinolinolato, or 2-methyl-8-quinolinolato and alkoxo = n butoxo or isopropoxo. In spite of the very wide range of electronic and steric properties of the phenoxy substituents, only complexes of cis stereochem. were obsd., and there seems little likelihood that complexes of this type can be induced to adopt a trans configuration. The dipole moments (D) and the relative chem. shifts (.DELTA..delta.) of the methine protons for a no. of



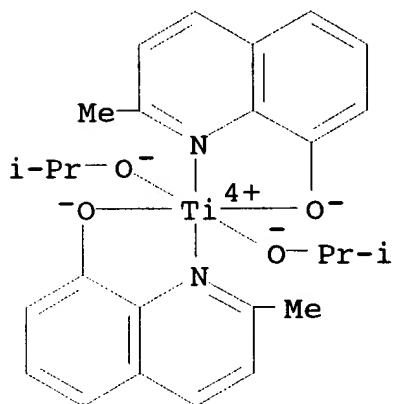
acetylacetonate complexes were measured. No systematic trends in the variation of .DELTA..delta. either with D or with the .rho.-parameters of the phenoxy ligands were obsd.

IT 33888-32-3 54516-87-9

(pren. and dipole moment of)

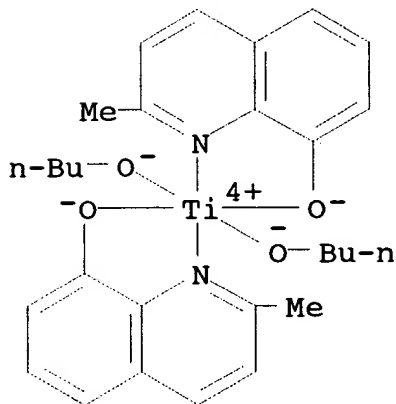
RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,O8)bis(2-propanolato)-(9CI) (CA INDEX NAME)



RN 54516-87-9 HCA

CN Titanium, dibutoxybis(2-methyl-8-quinolinolato-N1,O8)-(9CI) (CA INDEX NAME)

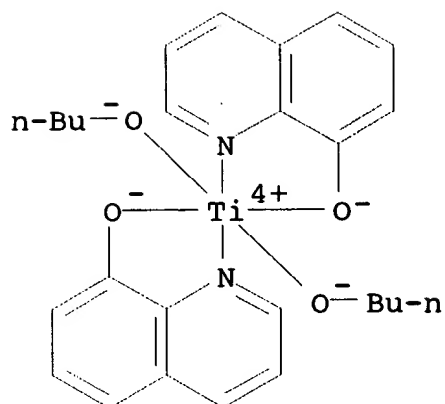


IT 17034-82-1P

(prepn. and dipole moments of)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)-(9CI) (CA INDEX NAME)

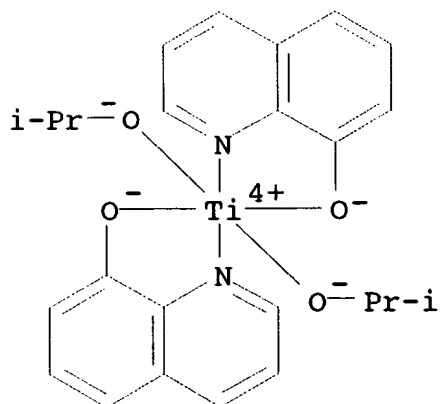


IT 23329-69-3P

(prepn. of)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 73IT 33888-31-2 33888-32-3 38781-12-3 54516-87-9  
(pren. and dipole moment of)IT 17034-82-1P 33939-16-1P 54516-88-0P 54516-91-5P  
54516-92-6P 54548-69-5P  
(prepn. and dipole moments of)IT 23329-69-3P 38781-13-4P 54516-89-1P 54516-90-4P  
54516-94-8P 54516-95-9P 54516-96-0P 54516-99-3P 54517-01-0P  
(prepn. of)

L38 ANSWER 31 OF 48 HCA COPYRIGHT 1998 ACS

83:70688 Preparation of quinolin-8-olates of titanium(III). Frazer, M.  
J.; Taylor, F. B.; Wilkins, T. A. (Dep. Chem., Polytech. North

London, London, Engl.). J. Inorg. Nucl. Chem., 37(3), 675-7 (English) 1975. CODEN: JINCAO.

AB Quinolin-8-ol (LH) with .alpha.-TiCl<sub>3</sub> and TiBr<sub>3</sub> in MeCN gave the quinolinolates TiXL<sub>2</sub> (I; X = Cl, Br) and the adduct TiCl<sub>3</sub>.2LH (II). TiL<sub>3</sub> with TiBr<sub>3</sub> in MeCN also gave TiBrL<sub>2</sub>. Redn. of TiClL<sub>3</sub> by Na in PhMe and of TiCl<sub>2</sub>L<sub>2</sub> by K in C<sub>6</sub>H<sub>6</sub> gave TiL<sub>3</sub> and TiClL<sub>2</sub>, resp. Reaction of I and II with dry O<sub>2</sub> gave (TiXL<sub>2</sub>)<sub>2</sub>O and [TiCl<sub>3</sub>(LH)<sub>2</sub>]<sub>2</sub>O, resp.

IT 56212-10-3P 56212-12-5P 56212-13-6P  
56212-15-8P

(prepn. of)

RN 56212-10-3 HCA

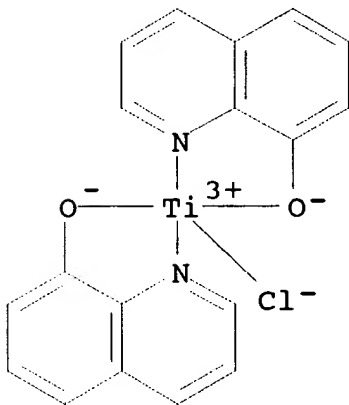
CN Titanium, chlorobis(8-quinolinolato-N1,O8)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 56212-09-0

CMF C18 H12 Cl N2 O2 Ti

CCI CCS



RN 56212-12-5 HCA

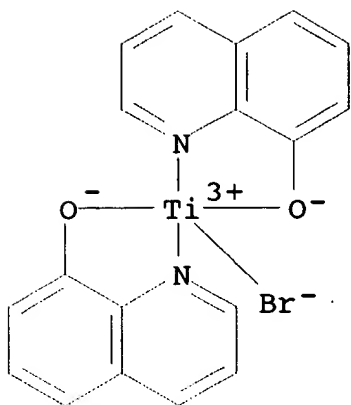
CN Titanium, bromobis(8-quinolinolato-N1,O8)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 56212-11-4

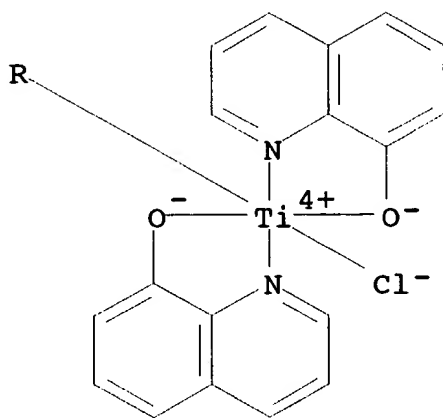
CMF C18 H12 Br N2 O2 Ti

CCI CCS

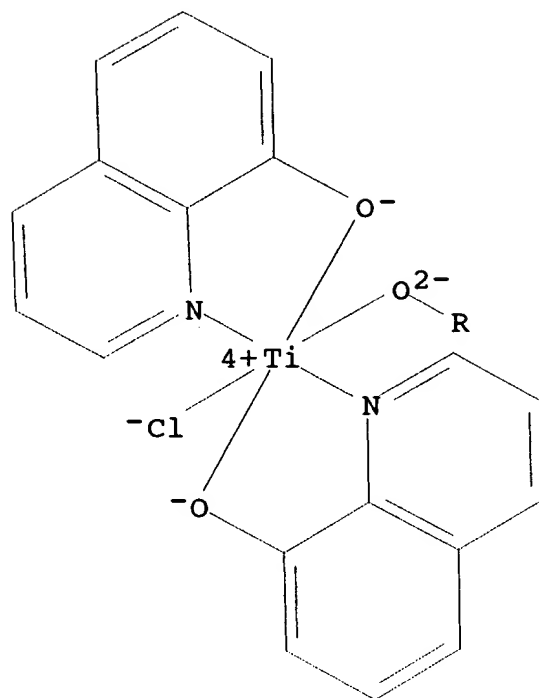


RN 56212-13-6 HCA  
CN Titanium, dichloro-.mu.-oxotetrakis(8-quinolinolato-N1,O8)di- (9CI)  
(CA INDEX NAME)

PAGE 1-A

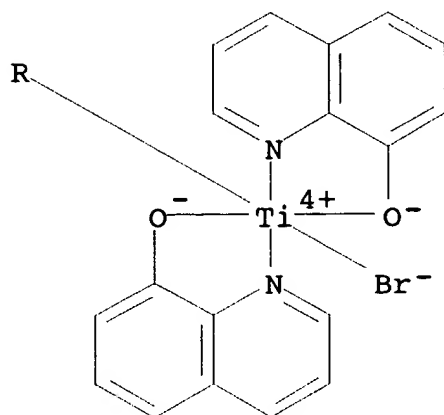


PAGE 2-A

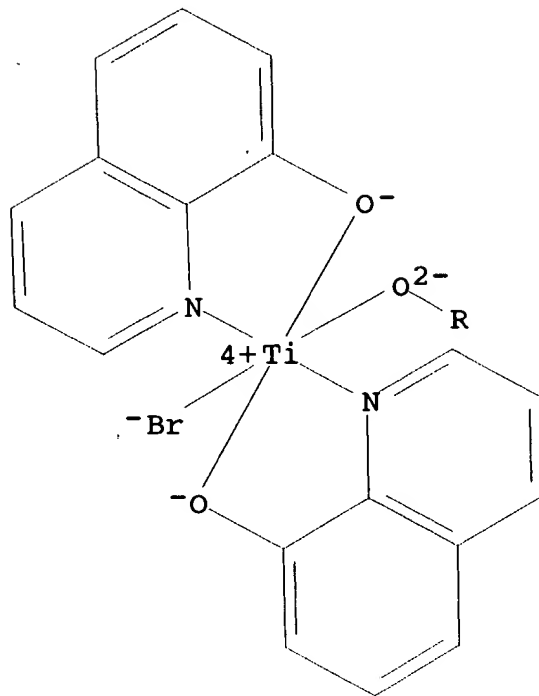


RN 56212-15-8 HCA  
 CN Titanium, dibromo-.mu.-oxotetrakis(8-quinolinolato-N1,O8)di- (9CI)  
 (CA INDEX NAME)

PAGE 1-A



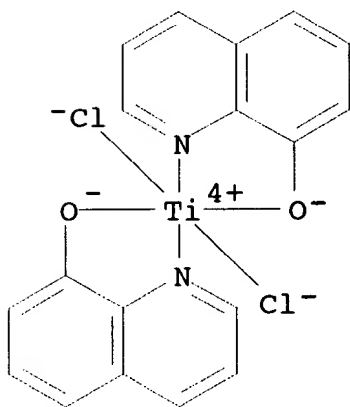
PAGE 2-A



IT 16905-40-1

(redn. of, by potassium)

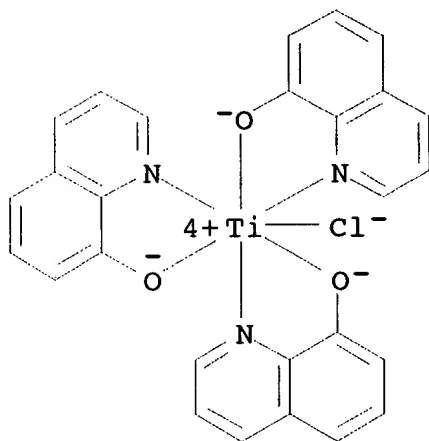
RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-κN1, κO8) - (9CI)  
(CA INDEX NAME)

IT 17442-90-9

(redn. of, by sodium)

RN 17442-90-9 HCA  
 CN Titanium, chlorotris(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
 (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

IT 56212-10-3P 56212-12-5P 56212-13-6P

56212-14-7P 56212-15-8P

(prepn. of)

IT 16905-40-1

(redn. of, by potassium)

IT 17442-90-9

(redn. of, by sodium)

L38 ANSWER 32 OF 48 HCA COPYRIGHT 1998 ACS

83:70081 Redistribution reactions in the ion source of a mass spectrometer of complexes of titanium(IV), tin(IV), and germanium(IV) with 8-quinolinolato and halo or ethoxy ligands. Barrett, C. G. R.; Charalambous, J.; Copperthwaite, R. G.; Frazer, M. J. (Polytech. North London, London, Engl.). Org. Mass Spectrom., 10(2), 146-54 (English) 1975. CODEN: ORMSBG.

AB In the mass spectra of MX<sub>2</sub>R<sub>2</sub> (M = Ge, Sn, Ti, X = F, Cl, Br, I, and R = 8-quinolinolato) and of Ti(OEt)<sub>4-n</sub>R<sub>n</sub> (n = 1, 2) redistribution reactions occurred to give ions of the type MX<sub>3</sub>R and MXR<sub>3</sub>. These reactions were confirmed by the variation in relative intensities of the peaks with insertion temp. and residence time of the sample in the spectrometer. The main fragmentation of MX<sub>2</sub>R<sub>2</sub> were loss of X or whole quinolinol radicals, reflecting the metal-halogen bond strength and the tendency of the metal to exist in low oxidn. states. Decompn. of Ti(OEt)<sub>3</sub>R and Ti(OEt)<sub>2</sub>R<sub>2</sub> involved loss of intact ligand radicals, whereas Ti(OEt)<sub>4</sub> also eliminated ligand fragments.

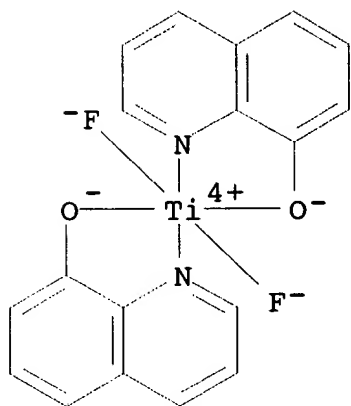
IT 16905-21-8 16905-40-1 16905-41-2

23329-68-2 56531-00-1

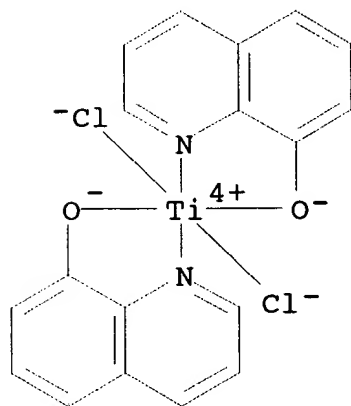
(mass spectrum of)

RN 16905-21-8 HCA

CN Titanium, difluorobis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



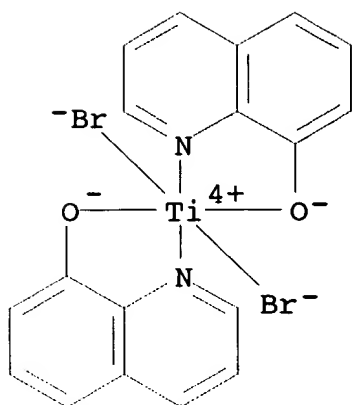
RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
(CA INDEX NAME)

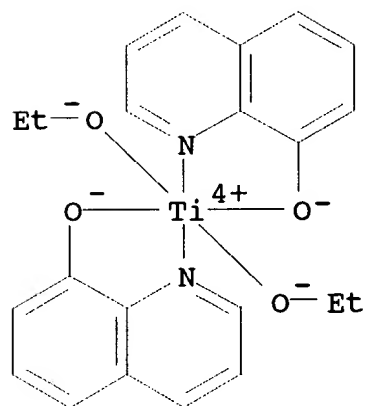
RN 16905-41-2 HCA

CN Titanium, dibromobis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

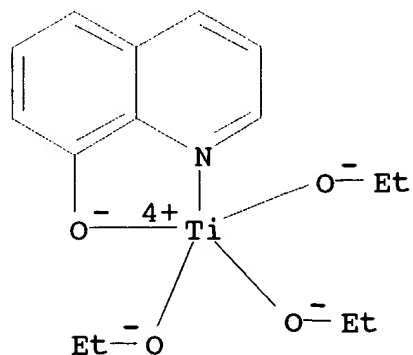




RN 23329-68-2 HCA  
CN Titanium, diethoxybis(8-quinolinolato-N1,O2)- (9CI) (CA INDEX NAME)

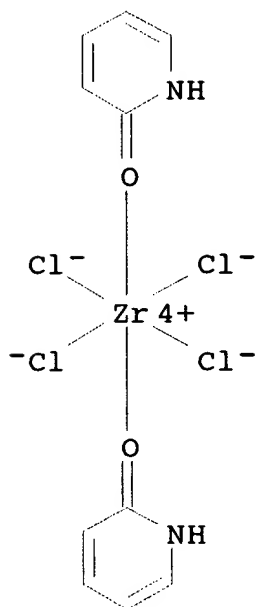


RN 56531-00-1 HCA  
CN Titanium, triethoxy(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 76-11 (Electric Phenomena)  
IT 3087-36-3 **16905-21-8** 16905-23-0 16905-24-1  
16905-25-2 16905-26-3 16905-35-4 **16905-40-1**  
**16905-41-2** 16925-43-2 **23329-68-2**  
**56531-00-1**  
(mass spectrum of)

L38 ANSWER 33 OF 48 HCA COPYRIGHT 1998 ACS  
79:119046 Heats of addition of pyridine and its derivatives to zirconium tetrachloride. Konunova, Ts. B.; Frunze, M. F. (Kishinev. Politekh. Inst. im. Lazo, Kishinev, USSR). Zh. Neorg. Khim., 18(7), 1800-5 (Russian) 1973. CODEN: ZNOKAQ.  
AB Heats of adduct formation of  $ZrCl_4$  with .alpha.-, .beta.-, o-picoline, .alpha.,.alpha.'-lutidine, .alpha.- and .beta.-chloropyridine, .gamma.-aminopyridine, .alpha.-amino-5-bromopyridine, .alpha.-pyridone, .beta.-benzoylpyridine, and .alpha.,.alpha.'-dipyridyl were detd. The heats of addn. of gaseous pyridine derivs. to anhyd.  $ZrCl_4$  are calcd. The heats become increasingly more neg. with an increasing pKa value of the amines.  
IT **37266-35-6P**  
(formation and heat of soln. of, in aq. hydrochloric acid)  
RN 37266-35-6 HCA  
CN Zirconium, tetrachlorobis(2(1H)-pyridinone)- (9CI) (CA INDEX NAME)



CC 69-1 (Thermodynamics, Thermochemistry, and Thermal Properties)  
Section cross-reference(s): 78  
IT 17100-06-0P **37266-35-6P** 38294-43-8P 42720-65-0P  
42720-66-1P 42769-05-1P 46946-20-7P 46946-24-1P 46946-26-3P

51176-89-7P 51176-90-0P 51176-92-2P  
(formation and heat of soln. of, in aq. hydrochloric acid)

L38 ANSWER 34 OF 48 HCA COPYRIGHT 1998 ACS

78:111503 Organocyclotitanosiloxanes. Pakhomov, V. I.; Levin, B. B.; Fomina, N. I.; Maizner, I. M.; Malyukova, F. Sh.; Shesternina, L. A.; Portnaya, N. Kh. U.S.S.R. SU 362018 721213 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1972, 50(2), 53. (Russian). CODEN: URXXAF. APPLICATION: SU 710121.

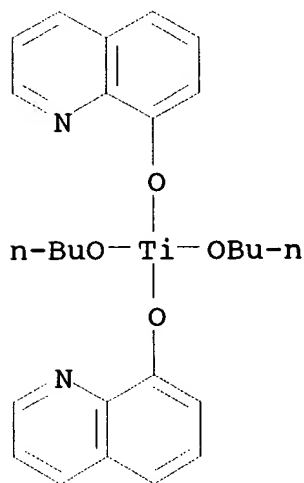
AB Organocyclotitanosiloxanes were prepd. by treating 3 equiv. of  $\text{Ph}_2\text{Si}(\text{OH})_2$  with 1 equiv. of bis(8-quinolinoxy)dibutoxytitanium in a solvent at 150-80.degree..

IT 41310-05-8

(reaction of, with dihydroxydiphenylsilane)

RN 41310-05-8 HCA

CN Titanium, dibutoxybis(8-quinolinolato-O)- (9CI) (CA INDEX NAME)



IC C07F

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 41310-05-8

(reaction of, with dihydroxydiphenylsilane)

L38 ANSWER 35 OF 48 HCA COPYRIGHT 1998 ACS

77:172052 Synthesis of complex compounds of zirconium and hafnium tetrahalides with primary amines. Konunova, Ts. B.; Frunze, M. F. (USSR). Tr. Tekhnol. Fak., Kishinev. Politekh. Inst., No. 24, 75-9 From: Ref. Zh., Khim. 1972, Abstr. No. 5V93 (Russian) 1971.

AB From Ref. Zh., Khim. 1972, Abstr. No. 5V93. The addn. of amine solns. in EtOAc to solns. of  $\text{ZrCl}_4$  in EtOAc gave the adducts  $\text{ZrCl}_4 \cdot n\text{L} \cdot m\text{EtOAc}$ , where n, L, and m are: 2, py, and 1 (I); 2, .alpha.-picoline (pic), and 0.5 (II); 2, .beta.-pic, and 0.5; 2, .gamma.-pic, and 0.5; 1.5, 3-benzylpyridine, and 1 (III); 2, 3-chloropyridine, and 0, 2, .alpha.-pyridone, and 0. I-III

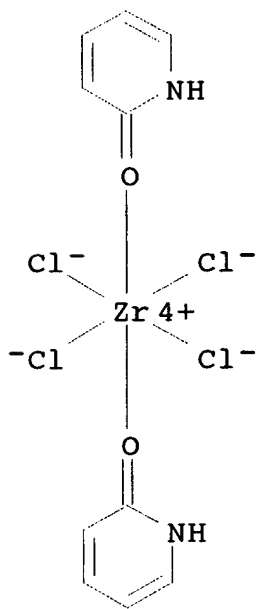
completely lost EtOAc at 100.degree.. The adducts  $\text{HfCl}_4 \cdot 2\text{L}$ , where L = py and .alpha.-pic, were also sepd. from solns. in EtOAc.  $\text{ZrCl}_4 \cdot 2(\text{iso-PrNH}_2) \cdot \text{EtOAc}$  and  $\text{ZrCl}_4 \cdot 4\text{EtNH}_2 \cdot 1.5\text{EtOAc}$  were obtained from solns. of  $\text{ZrCl}_4$  in EtOAc and solns. of amines in ether.  $\text{ZrCl}_4$  adducts with  $\text{PhNH}_2$  derivs. were sepd. from ether solns. These complexes were  $\text{ZrCl}_4 \cdot n\text{L}$ , where n and L are: 2 and  $\text{C}_7\text{H}_8\text{N}(\text{sic})$ ; 4 and  $\text{C}_7\text{H}_8\text{N}(\text{sic})$ ; 2 and  $\text{C}_7\text{H}_8\text{ON}(\text{sic})$ ; 4 and  $\text{C}_7\text{H}_8\text{ON}(\text{sic})$ ; 4 and p-toluidine.

IT 37266-35-6P

(prepn. of)

RN 37266-35-6 HCA

CN Zirconium, tetrachlorobis(2(1H)-pyridinone)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

IT 17100-02-6P 37266-35-6P 37266-85-6P 38293-32-2P  
 38293-33-3P 38293-34-4P 38293-35-5P 38294-43-8P 38296-88-7P  
 38442-04-5P 38442-05-6P 38448-78-1P  
 (prepn. of)

L38 ANSWER 36 OF 48 HCA COPYRIGHT 1998 ACS

77:36006 Organosilicon elastic compositions. Severnyi, V. V.;  
 Varlamova, N. V.; Minsker, E. I. Fr. FR 2076539 711119, 13 pp.  
 (French). CODEN: FRXXAK. APPLICATION: FR 70-1792 700119.

AB Elastomeric organosilicon compns. having improved heat resistance,  
 water resistance, and adhesion to metal substrates were prepd.  
 comprising .alpha.,.omega.-dihydroxypoly(diorganosiloxanes),  
 Si-contg. hardeners, and metal chelates. Thus, a homogeneous mixt.  
 of .alpha.,.omega.-dihydroxypoly(dimethylsiloxane),  $\text{ZnO}$ ,  
 bis(acetoacetate) dibutoxytitanium [16902-59-3], tetraethoxysilane  
 [78-10-4], and diethylaminomethyltriethoxysilane [15180-47-9] was

applied on a metal or org. glass substrate and cured at ambient temp. and 60% relative humidity to give an adherent film. Among the other metal chelates used were acetylacetatodiisopropoxyaluminum [19223-59-7] and bis(8-hydroxyquinoline) dibutoxytitanium [

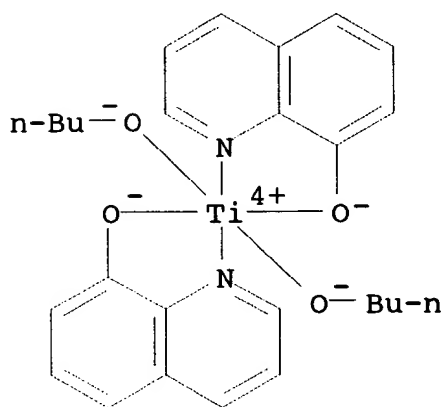
**17034-82-1**].

IT **17034-82-1**

(vulcanizing agents, contg. silanes, for silicone rubber)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



IC C08G; C09K

CC 38-9 (Elastomers, Including Natural Rubber)

IT 15710-92-6 16902-59-3 **17034-82-1** 19223-59-7  
38856-15-4

(vulcanizing agents, contg. silanes, for silicone rubber)

L38 ANSWER 37 OF 48 HCA COPYRIGHT 1998 ACS

76:142027 Physical properties of poly(organosiloxanes). II. Nonlinear and irregular poly(elementorganosiloxanes). Andrianov, K. A.; Slonimskii, G. L.; Zhdanov, A. A.; Levin, V. Yu.; Godovskii, Yu. K.; Moskalenko, V. A. (Inst. Organo-Elem. Compd., Moscow, USSR). J. Polym. Sci., Part A-1, 10(1), 23-43 (English) 1972. CODEN: JPLCAT.

AB Metal-contg. silicone rubber was prepd. by polymn. of siloxanes with aluminum butoxide [3085-30-1], tributoxy(8-quinolinolato)titanium [ **14843-25-5**], or halides of Zn, Pb, Ca, Cd, or Sn. The effect of compn., vulcanizatin, and fillers on the glass transition, melting and crystn. kinetics of the rubbers was detd.

IT **35277-47-5**

(silicone rubber contg., mech. properties of)

RN 35277-47-5 HCA

CC 38 (Elastomers, Including Natural Rubber)

IT 3085-30-1 **35277-47-5**

(silicone rubber contg., mech. properties of)

L38 ANSWER 38 OF 48 HCA COPYRIGHT 1998 ACS

75:110396 Reactions of 8-quinolinol with covalent halides. VI.

Bis- $\pi$ -cyclopentadienyldihalides of titanium, zirconium, and hafnium. Frazer, M. J.; Charalambous, J.; Newton, W. E. (Dep. Chem., North. Polytech., London, Engl.). J. Chem. Soc. A (15), 2487-91 (English) 1971. CODEN: JCSIAP.

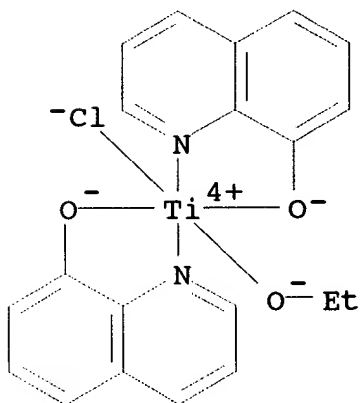
AB The complexes halocyclopentadienyldiquinolin-8-olatometal(IV),  $C_5H_5MX_2$  ( $M = Ti, Zr$ ;  $X = Cl, Br$  and  $M = Hf, X = Cl$ ), were prepd. by the direct interaction of quinolin-8-ol (oxH) and dihalobis (cyclopentadienyl)metal (IV)  $[(C_5H_5)_2MX_2]$  in acetonitrile soln. at room temp. Reactions of these complexes with ethanol, with ethoxide, and H halides were studied. Ir (4000-80  $cm^{-1}$ ), NMR, and mass spectra are reported.

IT 34090-33-0P 34765-99-6P

(prepn. of)

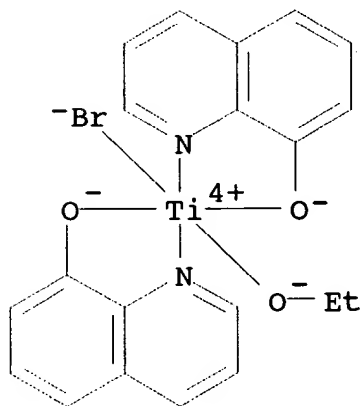
RN 34090-33-0 HCA

CN Titanium, chloroethoxybis(8-quinolinolato)- (8CI) (CA INDEX NAME)



RN 34765-99-6 HCA

CN Titanium, bromoethoxybis(8-quinolinolato)- (8CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 34090-33-0P 34765-99-6P

(prepn. of)

L38 ANSWER 39 OF 48 HCA COPYRIGHT 1998 ACS

75:67979 Intramolecular rearrangements in bis(chelate)titanium(IV) complexes. Harrod, J. F.; Taylor, K. (Chem. Dep., McGill Univ., Montreal, Que., Can.). J. Chem. Soc. D. (13), 696-7 (English) 1971. CODEN: CCJDAO.

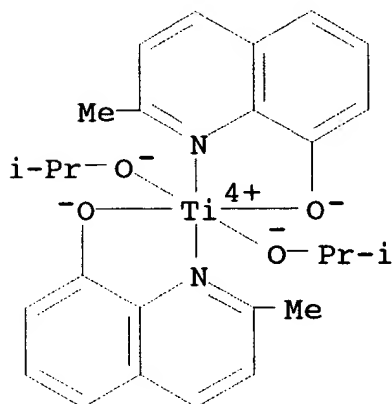
AB The rate of mol. rearrangement of bis(aryloxy)-bis(2,4-pentanedionato)titanium(IV) complexes (aryloxy = XC<sub>6</sub>H<sub>4</sub>O, X = p-Me, p-Ac, p-Cl, p-NO<sub>2</sub>, o-Me, o-iso-Pr, o-I, o-Cl) increases with decreasing pK<sub>a</sub> of the parent phenol, and the activation entropies for rearrangement are large and neg.

IT 33888-32-3

(nuclear magnetic resonance of, rearrangement in relation to)

RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,O8)bis(2-propanolato)-(9CI) (CA INDEX NAME)

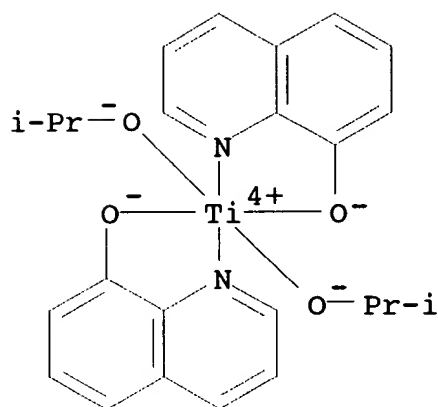


IT 23329-69-3

(rearrangement of, kinetics of)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,O8)-(9CI) (CA INDEX NAME)



CC 67 (Catalysis and Reaction Kinetics)

IT 33888-25-4 33888-26-5 33888-27-6 33888-28-7 33888-29-8  
 33888-30-1 33888-31-2 **33888-32-3** 33888-33-4  
 33939-16-1

(nuclear magnetic resonance of, rearrangement in relation to)

IT 17927-72-9 21324-45-8 **23329-69-3** 33887-44-4  
 33887-45-5 33887-46-6 33887-47-7 33887-48-8 33887-49-9  
 33887-50-2 33888-34-5

(rearrangement of, kinetics of)

L38 ANSWER 40 OF 48 HCA COPYRIGHT 1998 ACS

75:64782 Effectiveness of some poly(dimethylsiloxane) stabilizers.  
 Ditsent, V. E.; Skorokhodov, I. I.; Terent'eva, N. A.; Zolotareva,  
 M. N. (USSR). Sin. Issled. Eff. Khimikatov Polim. Mater., No. 3,  
 192-8 From: Ref. Zh., Khim. 1970, Abstr. No. 11S808 (Russian) 1969.

AB Twenty-four classes of compds. were studied as stabilizers against  
 thermal oxidative breakdown of .omega.,.omega.'-  
 hexamethyloligodimethylsiloxane. Organosilicone derivs. of  
 ferrocene, cyclopentadienylbenzoyltricarboxylmanganese and its  
 derivs., bis(8-hydroxyquinoline)dibutoxytitanium, and  
 4,4-dimethoxydiphenylamine are the most effective stabilizers, which  
 makes possible an increase of 60-70.degree. in the incipient  
 thermal-oxidative breakdown temp. of oligodimethylsiloxane.

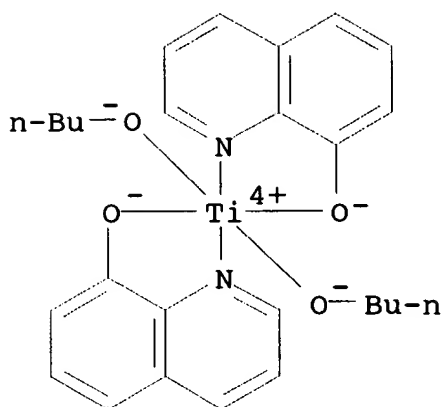
IT **17034-82-1**

(stabilizers, for siloxanes)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)





CC 36 (Plastics Manufacture and Processing)  
 IT 101-70-2 **17034-82-1** 33306-83-1  
 (stabilizers, for siloxanes)

L38 ANSWER 41 OF 48 HCA COPYRIGHT 1998 ACS

73:114013 Crystal and molecular structure of chloro- $\pi$ -cyclopentadienylbis(8-quinolinolato)titanium(IV). Matthews, James D.; Singer, N.; Swallow, Arnold G. (Dep. Chem., Northern Polytech., London, Engl.). J. Chem. Soc. A (15), 2545-9 (English) 1970. CODEN: JCSIAP.

AB The crystal and mol. structure of  $[\text{TiCl}(\pi\text{-C}_5\text{H}_5)(\text{C}_9\text{H}_6\text{NO})_2]$  has been detd. from 3-dimensional x-ray diffraction data. The unit cell is monoclinic with  $a = 8.82$ ,  $b = 13.85$ ,  $c = 16.80$  .ANG.,  $\beta = 111.7^\circ$ , and space group  $P2_1/c$ . The structure was solved by Patterson and Fourier methods from 2402 independent visually estd. intensities and refined by least-squares to  $R = 0.098$ . The structure consists of monomeric units with mol. geometry best described as dodecahedral but with certain similarities to a distorted octahedron. The O atoms lie in a trans-configuration, with respect to the octahedron, at 1.987 and 1.954 from the Ti, the N atoms cis at 2.224 and 2.270, and the Cl atom at 2.372 .ANG.. The long Ti-Cl distance and the differences between the Ti-O and Ti-N distances are discussed and compared with the corresponding distances in related compds.

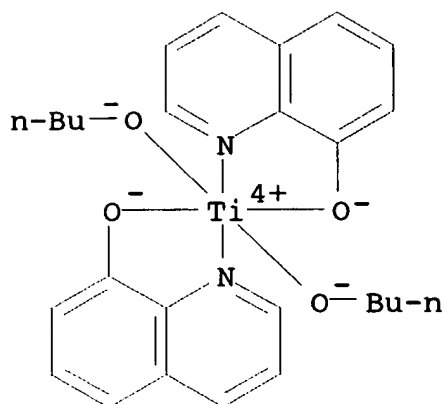
IT **31798-62-6**

(crystal structure of)

RN 31798-62-6 HCA

CN Titanium, chloro( $\eta$ -5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)





CC 35 (Synthetic High Polymers)

IT 17034-82-1P

(polymers with hydroxy-terminated methylphenylsiloxanes, prepn. of)

L38 ANSWER 43 OF 48 HCA COPYRIGHT 1998 ACS

70:53556 Titanium(IV) complexes with 8-quinolinol. Sen, D. N.; Umapathy, P. (Nat. Chem. Lab., Poona, India). J. Indian Chem. Soc., 45(11), 1006-11 (English) 1968. CODEN: JICSAH.

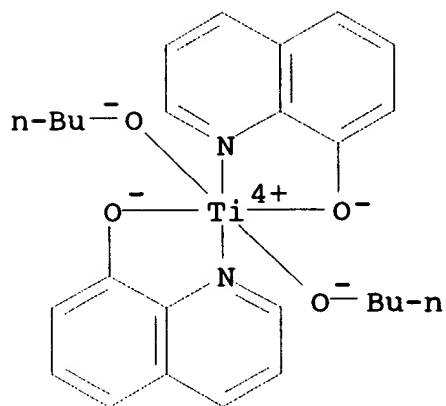
AB Ti(OR)<sub>2</sub>L<sub>2</sub>, where R = Et, iso-Pr, Bu, and HL = 8-quinolinol, were prepd. and studied. Titanoxane polymers were obtained by the hydrolysis of Ti(OR)<sub>2</sub>L<sub>2</sub> and of the reaction product of TiCl<sub>4</sub> with 8-quinolinol. Absorption bands due to alkoxy groups were absent in the ir spectra of the hydrolysis products of the dialkoxy compds. Strong and broad bands at .apprx.825 cm.<sup>-1</sup> and at .apprx.735 cm.<sup>-1</sup> ascribable to Ti-O-Ti stretching frequency were observed in the spectra of the hydrolysis products.

IT 17034-82-1P 23329-68-2P 23329-69-3P

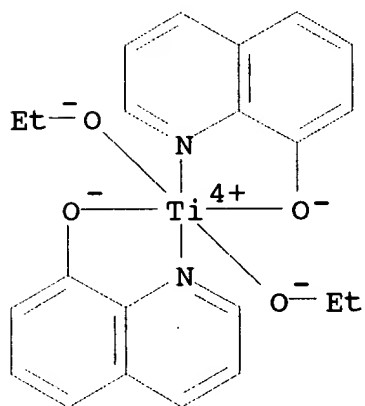
(prepn. of)

RN 17034-82-1 HCA

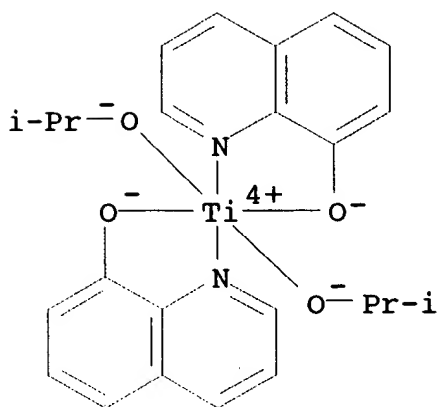
CN Titanium, dibutoxybis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



RN 23329-68-2 HCA  
CN Titanium, diethoxybis(8-quinolinolato-N1,O2)- (9CI) (CA INDEX NAME)



RN 23329-69-3 HCA  
CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)



CC 78 (Inorganic Chemicals and Reactions)

IT 17034-82-1P 22967-16-4P 22967-17-5P 23329-68-2P

23329-69-3P

(prepn. of)

L38 ANSWER 44 OF 48 HCA COPYRIGHT 1998 ACS

69:62437 Crystal and molecular structure of dichlorobis(8-quinolinolato)titanium(IV). Studd, B. F.; Swallow, A. G. (Dep. Chem., Northern Polytech., London, Engl.). J. Chem. Soc., A (8), 1961-7 (English) 1968. CODEN: JCSIAP.

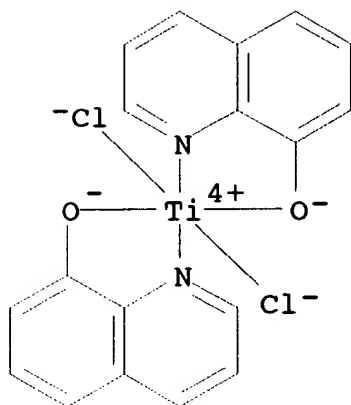
AB The crystal and mol. structure of  $\text{TiCl}_2(\text{C}_9\text{H}_6\text{NO})_2$  has been detd. by three-dimensional x-ray diffraction. The unit cell is monoclinic with  $a = 14.06$ ,  $b = 8.54$ ,  $c = 14.97$  A.,  $\beta = 111^\circ$ , and space group  $\text{C}2/c$ . The structure was solved by use of 1415 visually estd. intensities by Patterson and Fourier methods and refined by least sqs. to an R value of 0.116. The structure consists of monomeric units of  $\text{TiCl}_2(\text{Ox})_2$ , with two-fold symmetry, in which the Ti atom is octahedrally coordinated by two Cl atoms in a cis configuration, at a distance of 2.283, two N atoms also cis at 2.200, and two oxygen atoms in a trans configuration at 1.888 A. The large difference between the Ti-N and Ti-O distance is discussed and compared with distances in other metal-oxine complexes. 17 references.

IT 16905-40-1

(structure of)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
(CA INDEX NAME)



CC 70 (Crystallization and Crystal Structure)

IT 16905-40-1

(structure of)

L38 ANSWER 45 OF 48 HCA COPYRIGHT 1998 ACS

68:117788 Structure of dichlorodi-8-quinolinolatotitanium(IV). Swallow, Arnold G.; Studd, B. F. (Chem. Dep., Northern Polytech., London, Engl.). Chem. Commun. (23), 1197-8 (English) 1967. CODEN: CCOMA8.

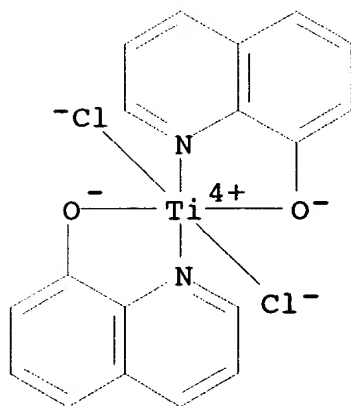
AB 8-Quinolinol (QOH) is treated with  $\text{TiCl}_4$  ( $\text{TiCl}_4$ :QOH molar ratio 1:2) to give  $\text{TiCl}_4 \cdot 2\text{QOH}$  (I); HCl is removed from I to give the title compd. (II), with a 14.06, b 8.54, c 14.97 Å, .beta. 111.degree. space group C2/c; dm is 1.64 and dc 1.61, Z = 4. II has a crystallographic 2-fold axis through the Ti atom, bisecting the Cl-Ti-Cl angle (97.degree.) and the N-Ti-N angle.

IT 16905-40-1

(crystal structure of)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
(CA INDEX NAME)



CC 70 (Crystallization and Crystal Structure)

IT 16905-40-1

(crystal structure of)

L38 ANSWER 46 OF 48 HCA COPYRIGHT 1998 ACS

67:82436 Coordination polymers of titanium(IV), tin(IV), and zirconium(IV). Sen, Dwijendra N.; Umapathy, P. (Natl. Chem. Lab., Poona, India). Indian J. Chem., 5(5), 209-10 (English) 1967. CODEN: IJOCAP.

AB The polymers were prepd. by adding  $TiCl_4$ ,  $Ti(OBu)_4$ ,  $Me_2SnCl_2$ , and  $ZrOCl_2 \cdot 8H_2O$  to heated solns. of bis(8-hydroxy-5-quinolyl)methane in  $HCONMe_2$ . Decompn. temps. for the Ti(IV), Zr(IV), and Sn(IV) polymers were 330.degree., 380.degree., and 410.degree., resp., indicating that thermal stability increased with at. no. of the metal. The polymer yields were 52.36, 97.5, 52.9, and 70%, resp., for  $TiCl_4$ ,  $Ti(OBu)_4$ ,  $Me_2SnCl_2$ , and  $ZrOCl_2$ .

IT 30972-50-0P

(prepn. of)

RN 30972-50-0 HCA

CN 8-Quinolinol, 5,5'-methylenedi-, polymer with titanium chloride ( $TiCl_3$ ) (8CI) (CA INDEX NAME)

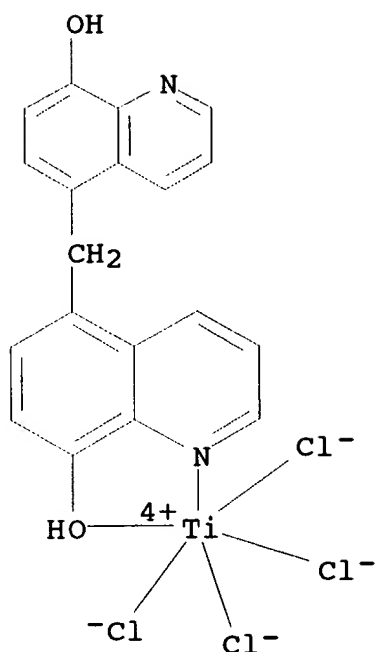
CM 1

CRN 52928-48-0

CMF C19 H14 Cl4 N2 O2 Ti

CCI CCS

CDES 7:OC-6-32



CC 35 (Synthetic High Polymers)  
 IT 30972-50-0P 30972-51-1P 31114-18-8P  
 (prepn. of)

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66:76121 Chemical transformations of dizirconoxane compounds.

Freidlina, R. Kh.; Brainina, E. M.; Petrashkevich, L. A.; Minacheva, M. Kh. (Inst. Hetero-Org. Compds., Moscow, USSR). Izv. Akad. Nauk SSSR, Ser. Khim. (8), 1396-9 (Russian) 1966. CODEN: IASKA6.

AB cf. CA 60, 12038g. Heating 0.018 g. H<sub>2</sub>O, 0.0896 g. abs. EtOH, 0.197 g. Et<sub>3</sub>N, 1.0 g. dibenzoylacetonatocyclopentadienylzirconium chloride and C<sub>6</sub>H<sub>6</sub> 1 hr. at 40-5.degree. gave after sepn. of Et<sub>3</sub>N.HCl 64% dicyclopentadienyldizirconoxane tetrabenzoylacetonate (I), [(C<sub>5</sub>H<sub>5</sub>)(C<sub>10</sub>H<sub>9</sub>O<sub>2</sub>)<sub>2</sub>Zr]<sub>2</sub>O, decompd. at 172-5.degree., which contained stubbornyl held C<sub>6</sub>H<sub>6</sub>. Similar reaction with bis - 8 - hydroxyquinolinocyclopentadienylzirconium chloride (prepd. from (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrCl<sub>2</sub> and 8-hydroxyquinoline in C<sub>6</sub>H<sub>6</sub>, m. 260-3.degree.), gave dicyclopentadienyldizirconoxane tetra-8-hydroxyquinolate (II), [(C<sub>5</sub>H<sub>5</sub>)(C<sub>9</sub>H<sub>6</sub>ON)<sub>2</sub>Zr]<sub>2</sub>O, infusible at 300.degree.. Adding p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H in tetrahydrofuran to [(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrCl]<sub>2</sub>O at 5.degree. gave in 2 hrs. 50% (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrCl(O<sub>3</sub>SC<sub>6</sub>H<sub>4</sub>Me-p).H<sub>2</sub>O, m. 166-9.degree.; similar reaction with concd. H<sub>2</sub>SO<sub>4</sub> in (CH<sub>2</sub>Cl)<sub>2</sub> gave 62% (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Zr(OSO<sub>3</sub>H)<sub>2</sub>.4H<sub>2</sub>O, infusible and hygroscopic solid; similarly HNO<sub>3</sub> gave (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrClNO<sub>3</sub>, m. 190.5.degree.. Reaction of HNO<sub>3</sub> (d. 135) in (CH<sub>2</sub>Cl)<sub>2</sub> with dicyclopentadienylzirconium dichloride at -30.degree., followed by 1 hr. at room temp., gave 62% (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrCl(NO<sub>3</sub>), m. 190.degree., as above. Reaction of



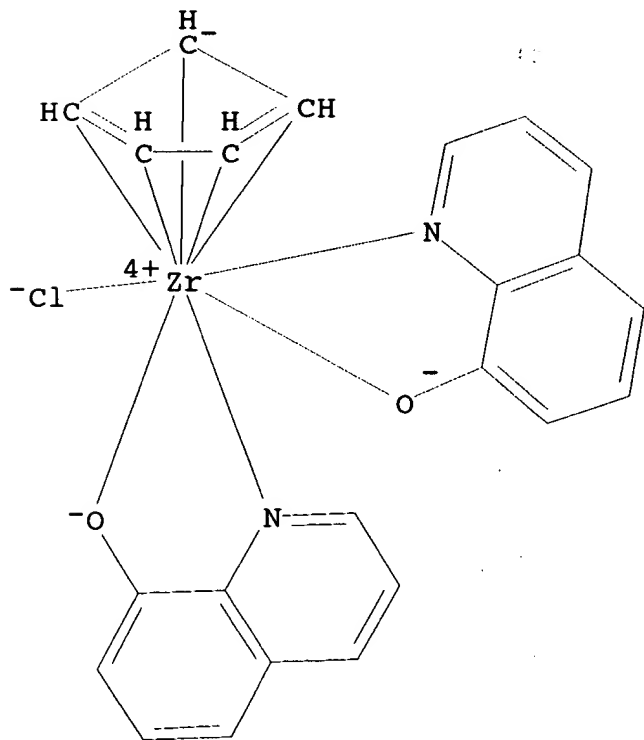
p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H with dicyclopentadienyldizirconoxane tetraacetyl-acetate in tetrahydrofuran, finally at 40.degree., gave 77% (C<sub>5</sub>H<sub>5</sub>) (C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>Zr(O<sub>3</sub>SC<sub>6</sub>H<sub>4</sub>Me-p).0.5C<sub>4</sub>H<sub>8</sub>O, m. 187.5-90.degree. (from tetrahydrofuran); HNO<sub>3</sub> similarly gave 47% (C<sub>5</sub>H<sub>5</sub>) (C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>Zr(NO<sub>3</sub>), m. 137-40.degree.. Heating CH<sub>2</sub>Bz<sub>2</sub> with tetracyclopentadienyldizirconoxane dichloride at 100-10.degree. 40 min. gave 45% (C<sub>15</sub>H<sub>11</sub>O<sub>2</sub>)<sub>2</sub>ZrCl(C<sub>5</sub>H<sub>5</sub>) decompd. at 225-7.degree.; similarly 8-hydroxyquinoline gave (C<sub>9</sub>H<sub>6</sub>ON)<sub>2</sub>ZrCl(C<sub>5</sub>H<sub>5</sub>), m. 260-3.degree.. Bz<sub>2</sub>CH<sub>2</sub> and (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>ZrCl<sub>2</sub> at 90.degree. in C<sub>6</sub>H<sub>6</sub> in vacuo 22 hrs. gave 65% bis(dibenzoylmethanocyclopentadienyl)zirconium chloride, decompd. at 224-6.degree.; similar reaction with 8-hydroxyquinoline gave 76% bis(8-hydroxyquinolate) of cyclopentadienylzirconium chloride, (C<sub>9</sub>H<sub>6</sub>ON)<sub>2</sub>ZrCl(C<sub>5</sub>H<sub>5</sub>), m. 260-3.degree.. The above reactions illustrated the basic nature of the dizirconoxane group.

IT 12114-15-7P

(prepn. of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 12111-83-0P 12114-03-3P 12114-15-7P 12116-65-3P

12119-26-5P 12121-09-4P 12124-07-1P 12193-45-2P 12193-84-9P

(prepn. of)

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66:70504 Far infrared spectra of some compounds of Group IV tetrahalides with 8-quinolinol, salicylaldehyde, and acetylacetone. Douek, I.; Frazer, Malcolm J.; Goffer, Z.; Goldstein, Michael; Rimmer, B.; Willis, Harry A. (Northern Polytech., London, Engl.). Spectrochim. Acta, 23A(2), 373-81 (English) 1967. CODEN: SPACA5.

AB The far ir spectra (450-80  $\text{cm}^{-1}$ ) of several complexes of the type  $\text{MX}_2\text{ke}_2$ ,  $\text{MX}_4.2\text{keH}$ , and  $\text{MX}_4.\text{keH}$  ( $\text{M} = \text{Ti}, \text{Zr}, \text{Ge}, \text{or Sn}$ ;  $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{or I}$ ;  $\text{keH} = 8\text{-quinolinol}, \text{salicylaldehyde}, \text{or acetylacetone}$ ) have been studied. Vibrations involving metal-halogen stretching have been assigned, and suggestions made as to the likely stereochem. configurations of some of the compds., but because of the complexity of the spectra and other factors discussed, it has not been possible to establish configurations unequivocally. Possibly the complexes  $\text{TiCl}_4.(8\text{-quinolinol})$  and  $\text{SnCl}_4.(8\text{-quinolinol})$  are monomeric, 5-coordinate species in the solid state. For analogous compds., the relation  $\frac{\nu(\text{SnX})}{\nu(\text{TiX})} \approx 0.90$  is independent of the halogen and other ligands, and applies to all the compds. now studied as well as to those previously reported in the literature. 37 references.

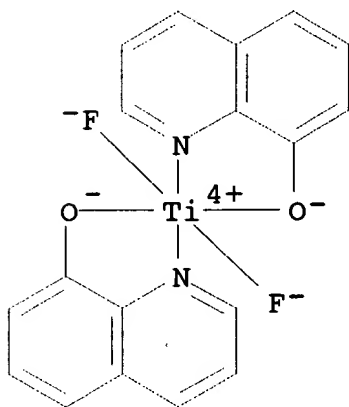
IT 16905-21-8 16905-40-1 19032-85-0

19049-15-1 19381-58-9

(spectrum (ir) of)

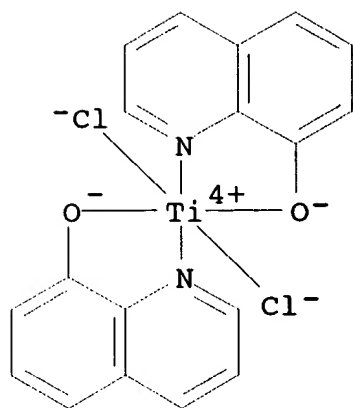
RN 16905-21-8 HCA

CN Titanium, difluorobis(8-quinolinolato-N1,O8)- (9CI) (CA INDEX NAME)

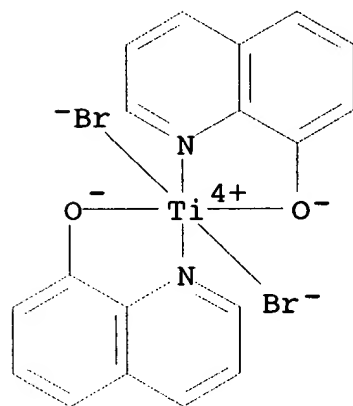


RN 16905-40-1 HCA

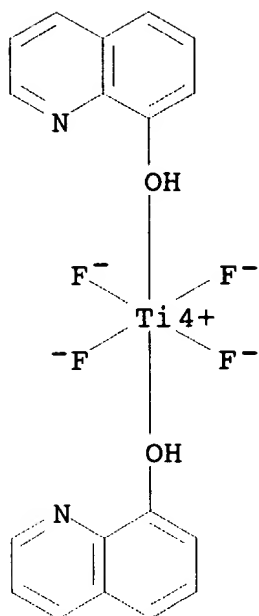
CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)  
(CA INDEX NAME)



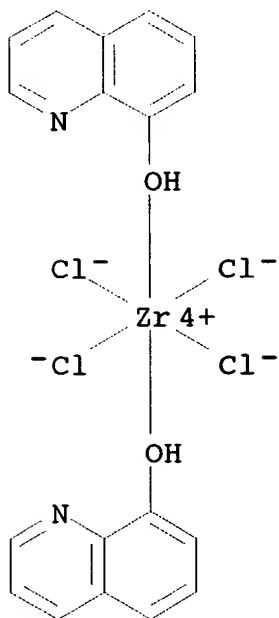
RN 19032-85-0 HCA  
 CN Titanium, dibromobis(8-quinolinolato)-, trans- (8CI) (CA INDEX NAME)



RN 19049-15-1 HCA  
 CN Titanium, tetrafluorobis(8-quinolinol)- (8CI) (CA INDEX NAME)



RN 19381-58-9 HCA  
CN Zirconium, tetrachlorobis(8-quinolinol)- (8CI) (CA INDEX NAME)



CC 73 (Spectra and Other Optical Properties)  
IT 148-24-3, properties 15523-68-9 **16905-21-8** 16905-24-1

16905-25-2	16905-26-3	16905-27-4	16905-35-4	<b>16905-40-1</b>
16905-42-3	16919-65-6	16919-66-7	16919-67-8	16925-43-2
17029-26-4	17099-86-4	17185-49-8	17218-25-6	<b>19032-85-0</b>
<b>19049-15-1</b>	19154-04-2	19154-08-6	19154-09-7	
19154-10-0	19154-11-1	19154-12-2	19154-13-3	19154-16-6
19154-17-7	<b>19381-58-9</b>	19978-93-9		

(spectrum (ir) of)